LIST OF 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*, edited by J. Leszczynski (World Scientific, Singapore, 2000), Vol. 5, pp. 1-104 [monograph, invited book chapter].
6.* P. Piecuch, K. Kowalski, I.S.O. Pimienta, and S.A. Kucharski, "Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing "Black-Box" Approaches for Molecular Potential Energy Surfaces," in: *Low-Lying Potential Energy Surfaces*, ACS Symposium Series, Vol. 828, edited by M.R. Hoffmann and K.G. 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 $**$

[††] 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).
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. Toboła, and J. Paldus, "Approximate Account of Connected Quadruply Excited Clusters in Multi-Reference Hilbert Space Coupled-Cluster Theory. Application to Planar H_4 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. Szczęśniak, G. Chałasiński, and P. Piecuch, "The Nonadditive Interactions in the Ar_2HF and Ar_2HCl 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 $(H_2)_2$ 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 H_8 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 H_8," *Chem. Phys. Lett.* **221**, 121-128 (1994).

58. X. Li, P. Piecuch, and J. Paldus, "A Study of $^1A_1 - {}^3B_1$ Separation in CH_2 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 $^1A_1 - {}^3B_1$ Energy Gap in CH_2 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).

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 H_8," *J. Chem. Phys.* **102**, 3301-3306 (1995).

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).
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 Semi-internal Triexcited Clusters: Potential Energy Surface of the 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 N_2. 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 N_2. II. Rovibrational Effects," *J. Chem. Phys.* **104**, 4716-4727 (1996).
69. K.B. Ghose, P. Piecuch, S. Pal, and L. Adamowicz, "State-Selective Multireference 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 CH_3F^- Anions: A Coupled Cluster Study," *J. Mol. 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. $Na \cdots FH$," *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.

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 Quasi-degenerate 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 Kołos; 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. Bludský, "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 N_2 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. Sekušak, 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. Bludský, "Lifetimes and Dissociation Pathways of Quasi-Bound States of the Na$\cdots$FH van der Waals Molecule," *J. Mol. 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. Bludský, "Bound and Quasi-Bound States of the Li$\cdots$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. Li$\cdot\cdot$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. Füzéry, 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. Mol. 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. Bludský, "Bound and Quasi-Bound States of the Li$\cdots$FH van der Waals Molecule: The Effect of the Potential Energy Surface and of the Basis Set Superposition Error," *J. Mol. 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, "Non-iterative 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 Cu_2O_2 Torture Track. Mechanistic Implications for Oxytyrosinase and Small-Molecule Analogues," *J. Phys. Chem. A* **110**, 1991-2004 (2006); *ibid.* **111**, 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 Acetyloacetone 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 ^{16}O," *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 (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, "Stereoelectronic 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 $H_2S(^1A')$ 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 $V_{\rm UCOM}$ 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. Wesołowski, 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, C_2N, N_3, 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 Kinetic 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. DeYonker, 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. Kozlowski, 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. Kozlowski, "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 Au_8: 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 Au_8^-: 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 Au_3^-," *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: $Mg_n^{0,\pm1}$, $n = 1 - 7$," *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 Ag_3^-," *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.* **117**, 1486-1506 (2019) [Special Memorial Issue in Honour of Professor Dieter Cremer; invited contribution; in response to an invitation issued to P. Piecuch].

210.** J.E. Deustua, S.H. Yuwono, J. Shen, and P. Piecuch, "Communication: Accurate Excited-State Energetics by a Combination of Monte Carlo Sampling and Equation-of-Motion Coupled-Cluster Computations," *J. Chem. Phys.* **150**, 111101-1 – 111101-7 (2019).

211.** J. Lahiri, M. Moemeni, J. Kline, B. Borhan, I. Magoulas, S.H. Yuwono, P. Piecuch, J.E. Jackson, M. Dantus, and G.J. Blanchard, "Proton Abstraction Mediates Interactions Between the Super Photobase FR0-SB and Surrounding Alcohol Solvent," *J. Phys. Chem. B* **123**, 8448-8456 (2019).

212.** S.H. Yuwono, I. Magoulas, and P. Piecuch, "Quantum Computation Solves a Half-Century-Old Enigma: Elusive Vibrational States of Magnesium Dimer Found," *Sci. Adv.* **6**, eaay4058 (2020).

213.** G.M.J. Barca, C. Bertoni, L. Carrington, D. Datta, N. De Silva, J.E. Deustua, D.G. Fedorov, J.R. Gour, A.O. Gunina, E. Guidez, T. Harville, S. Irle, J. Ivanic, K. Kowalski, S.S. Leang, H. Li, W. Li, J.J. Lutz, I. Magoulas, J. Mato, V. Mironov, H. Nakata, B.Q. Pham, P. Piecuch, D. Poole, S.R. Pruitt, A.P. Rendell, L.B. Roskop, K. Ruedenberg, T. Sattasathuchana, M.W. Schmidt, J. Shen, L. Slipchenko, M. Sosonkina, V. Sundriyal, A. Tiwari, J.L.G. Vallejo, B. Westheimer, M. Włoch, P. Xu, F. Zahariev, and M.S. Gordon, "Recent Developments in the General Atomic and Molecular Electronic Structure System," *J. Chem. Phys.* **152**, 154102-1 – 154102-26 (2020) [Special Topic Collection "Electronic Structure Software"; invited contribution].

214.** K.A. O'Hearn, M.W. Swift, J. Liu, I. Magoulas, P. Piecuch, A.C.T. van Duin, H.M. Aktulga, and Y. Qi, "Optimization of the Reax Force Field for Lithium Dioxide using a High Fidelity Charge Model," *J. Chem. Phys.* **153**, 084107-1 – 084107-10 (2020) [Special Topic Collection "Classical Molecular Dynamics (MD) Simulations: Codes, Algorithms, Force Fields, and Applications"; invited contribution].

215.** J. Lahiri, M. Moemeni, I. Magoulas, S.H. Yuwono, J. Kline, B. Borhan, P. Piecuch, J.E. Jackson, G.J. Blanchard, and M. Dantus, "Steric Effects in Light-Induced Solvent Proton Abstraction," *Phys. Chem. Chem. Phys.* **22**, 19613-19622 (2020).

216.** S.H. Yuwono, A. Chakraborty, J.E. Deustua, J. Shen, and P. Piecuch, "Accelerating Convergence of Equation-of-Motion Coupled-Cluster Computations Using the Semi-Stochastic CC(P;Q) Formalism," *Mol. Phys.* **118**, e1817592 (2020), 17 pages [Special Issue in Honour of Professor Jürgen Gauss; invited contribution; in response to an invitation issued to P. Piecuch].

217.** J.R. Reimers, J. Shen, M. Kianinia, C. Bradac, I. Aharonovich, M.J. Ford, and P. Piecuch, "Photoluminescence, Photophysics, and Photochemistry of the V_B^- Defect in Hexagonal Boron Nitride," *Phys. Rev. B* **102**, 144105-1 – 144105-17 (2020).

218.** J.J. Eriksen, T.A. Anderson, J.E. Deustua, K. Ghanem, D. Hait, M.R. Hoffmann, S. Lee, D.S. Levine, I. Magoulas, J. Shen, N.M. Tubman, K.B. Whaley, E. Xu, Y. Yao, N. Zhang, A. Alavi, G.K.-L. Chan, M. Head-Gordon, W. Liu, P. Piecuch, S. Sharma, S.L. Ten-no, C.J. Umrigar, and J. Gauss "The Ground State Electronic Energy of Benzene," *J. Phys. Chem. Lett.* **11**, 8922-8929 (2020).

219.** J. Lahiri, M. Moemeni, J. Kline, I. Magoulas, S.H. Yuwono, M. Laboe, J. Shen, B. Borhan, P. Piecuch, J.E. Jackson, G.J. Blanchard, and M. Dantus, "Isoenergetic Two-Photon Excitation Enhances Solvent-to-Solute Excited-State Proton Transfer," *J. Chem. Phys.* **153**, 224301-1 – 224301-14 (2020).

220.** J.E. Deustua, J. Shen, and P. Piecuch, "High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions: Further Details and Comparisons," *J. Chem. Phys.* **154**, 124103-1 – 124103-25 (2021) [Special Topic Collection

"Frontiers of Stochastic Electronic Structure Calculations"; invited contribution; in response to an invitation issued to P. Piecuch].

221.** I. Magoulas, K. Gururangan, P. Piecuch, J.E. Deustua, and J. Shen, "Is Externally Corrected Coupled Cluster Always Better than the Underlying Truncated Configuration Interaction?," *J. Chem. Theory Comput.* **17**, 4006-4027 (2021).

222.** J. Lahiri, S.H. Yuwono, I. Magoulas, M. Moemeni, B. Borhan, G.J. Blanchard, P. Piecuch, and M. Dantus, "Controlling Quantum Interference between Virtual and Dipole Two-Photon Optical Excitation Pathways Using Phase-Shaped Laser Pulses," *J. Phys. Chem. A* **125**, 7534-7544 (2021).

223.** J. Shen and P. Piecuch, "Double Electron-Attachment Equation-of-Motion Coupled-Cluster Methods with up to 4-particle–2-hole Excitations: Improved Implementation and Application to Singlet–Triplet Gaps in *ortho*-, *meta*-, and *para*-Benzyne Isomers," *Mol. Phys.* **119**, e1966534 (2021), 18 pages [Special Issue in Honour of Professor John F. Stanton (John Stanton Special Issue: Theory Meets Experiment); invited contribution; in response to an invitation issued to P. Piecuch].

224.** W. Park, J. Shen, S. Lee, P. Piecuch, M. Filatov, and C.H. Choi, "Internal Conversion between Bright ($1^1B_u^+$) and Dark ($2^1A_g^-$) States in s-*trans*-Butadiene and s-*trans*-Hexatriene," *J. Phys. Chem. Lett.* **12**, 9720-9729 (2021).

225.** K. Gururangan, J.E. Deustua, J. Shen, and P. Piecuch, "High-Level Coupled-Cluster Energetics by Merging Moment Expansions with Selected Configuration Interaction," *J. Chem. Phys.* **155**, 174114-1 – 174114-14 (2021).

226.** B.A. Capistran, S.H. Yuwono, M. Moemeni, S. Maity, A. Vahdani, B. Borhan, J.E. Jackson, P. Piecuch, M. Dantus, and G.J. Blanchard, "Excited State Dynamics of a Substituted Fluorene Derivative. The Central Role of Hydrogen Bonding Interactions with the Solvent," *J. Phys. Chem. B* **125**, 12242-12253 (2021).

227.** B.A. Capistran, S.H. Yuwono, M. Moemeni, S. Maity, A. Vahdani, B. Borhan, J.E. Jackson, P. Piecuch, M. Dantus, and G. J. Blanchard, "Intramolecular Relaxation Dynamics Mediated by Solvent-Solute Interactions of Substituted Fluorene Derivatives. Solute Structural-Dependence," *J. Phys. Chem. B* **125**, 12486-12499 (2021).

228.** I. Magoulas, J. Shen, and P. Piecuch, "Addressing Strong Correlation by Approximate Coupled-Pair Methods with Active-Space and Full Treatments of Three-Body Clusters," *Mol. Phys.* **120**, e2057365 (2022), 30 pages [Special Issue in Memory of Professor Lutosław Wolniewicz (L. Wolniewicz Special Issue); invited contribution; in response to an invitation issued to P. Piecuch].

229.** W. Park, J. Shen, S. Lee, P. Piecuch, T. Joo, M. Filatov (Gulak), and C.H. Choi, "Dual Fluorescence of Octatetraene Hints at a Novel Type of Singlet–to–Singlet Thermally Activated Delayed Fluorescence Process," *J. Phys. Chem. C* **126**, 14976-14985 (2022).

230.** A. Chakraborty, S.H. Yuwono, J.E. Deustua, J. Shen, and P. Piecuch, "Benchmarking the Semi-Stochastic CC(P;Q) Approach for Singlet–Triplet Gaps in Biradicals," *J. Chem. Phys.* **157**, 134101-1 – 134101-23 (2022) [Special Topic Collection "Nature of the Chemical Bond"; invited contribution; in response to an invitation issued to P. Piecuch].

231.** A.M. Teale, T. Helgaker, A. Savin, C. Adamo, B. Aradi, A.V. Arbuznikov, P.W. Ayers, E.J. Baerends, V. Barone, P. Calaminici, E. Cancès, E.A. Carter, P.K. Chattaraj, H. Chermette, I. Ciofini, T.D. Crawford, F. De Proft, J.F. Dobson, C. Draxl, T. Frauenheim, E. Fromager, P. Fuentealba, L. Gagliardi, G. Galli, J. Gao, P. Geerlings, N. Gidopoulos, P.M.W. Gill, P. Gori-Giorgi, A. Görling, T. Gould, S. Grimme, O. Gritsenko, H.J.A. Jensen, E.R. Johnson, R.O. Jones, M. Kaupp, A.M. Köster, L. Kronik, A.I. Krylov, S. Kvaal, A. Laestadius, M. Levy, M. Lewin, S. Liu, P.-F. Loos, N.T. Maitra, F. Neese, J.P. Perdew, K. Pernal, P. Pernot, P. Piecuch, E. Rebolini, L. Reining, P. Romaniello, A. Ruzsinszky, D.R. Salahub, M. Scheffler, P. Schwerdtfeger, V.N. Staroverov, J. Sun, E. Tellgren, D.J. Tozer, S.B. Trickey, C.A. Ullrich, A. Vela, G. Vignale, T.A. Wesołowski, X. Xu, and W. Yang, "DFT Exchange: Sharing Perspectives on the Workhorse of Quantum Chemistry and Materials Science," *Phys. Chem. Chem. Phys.* **24**, 28700-28781 (2022) [PCCP Perspective, Themed Collection PCCP Reviews; invited contribution].

232.** J. Stamm, S. Li, B. Jochim, S.H. Yuwono, S.S. Priyadarsini, P. Piecuch, and M. Dantus, "Femtosecond Intramolecular Rearrangement of the CH_3NCS Radical Cation," *J. Chem. Phys.* **157**, 214304-1 – 214304-8 (2022).

233.** F. Zahariev, P. Xu, B.M. Westheimer, S. Webb, J.G. Vallejo, A. Tiwari, V. Sundriyal, M. Sosonkina, J. Shen, G. Schoendorff, M. Schlinsog, T. Sattasathuchana, K. Ruedenberg, L.B. Roskop, A.P. Rendell, D. Poole, P. Piecuch, B.Q. Pham, V. Mironov, J. Mato, S. Leonard, S.S. Leang, J. Ivanic, J. Hayes, T. Harville, K. Gururangan, E. Guidez, I.S. Gerasimov, C. Friedl, K.N. Ferreras, G. Elliott, D. Datta, D. Del Angel Cruz, L. Carrington, C. Bertoni, G.M.J. Barca, M. Alkan, and M.S. Gordon, "The General Atomic and Molecular Electronic Structure System (GAMESS): Novel Methods on Novel Architectures," *J. Chem. Theory Comput.* **19**, 7031-7055 (2023) [Special Issue "Electronic Structure Theory Packages of Today and Tomorrow"; invited contribution].

234.** K. Gururangan and P. Piecuch, "Converging High-Level Coupled-Cluster Energetics via Adaptive Selection of Excitation Manifolds Driven by Moment Expansions," *J. Chem. Phys.* **159**, 084108-1 – 084108-16 (2023).

235.** J. Stamm, S.S. Priyadarsini, S. Sandhu, A. Chakraborty, J. Shen, S. Kwon, J. Sandhu, C. Wicka, A. Mehmood, B.G. Levine, P. Piecuch, and M. Dantus, "H_3^+ Formation from Methyl Halogens and Pseudohalogens: Experiment, Theory, and Governing Factors," *Nat. Commun.*, resubmitted after revision (2024).

236.** S.S. Priyadarsini, K. Gururangan, J. Shen, and P. Piecuch, "The Singlet–Triplet Gap of Cyclobutadiene: The CIPSI-Driven CC(P;Q) Study," *J. Phys. Chem. A*, submitted (2024); in revision [Virtual Special Issue in honor of Professor Gustavo E. Scuseria ("Gustavo Scuseria Festschrift"); invited contribution; in response to an invitation issued to P. Piecuch].

LIST OF EDITED JOURNAL ISSUES AND BOOKS[†]

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.

[†] Excluding memberships of editorial boards, which are listed in section Editorial Boards of Curriculum Vitae.

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.

LIST OF INVITED TALKS AT INTERNATIONAL, NATIONAL, AND REGIONAL SYMPOSIA[†]

1. "Application of the Hilbert-Space Coupled-Cluster Theory to Electronic States of the H_4 Model System," Workshop "Coupled Clusters in the Theory of Atoms and Molecules," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Warsaw, Poland, October 23-24, 1992.

2. "Linear Response Coupled-Cluster Approach to Static Molecular Properties," The symposium "Frontiers in Electronic Structure Theory," 213th American Chemical Society National Meeting, San Francisco, California, U.S.A., April 13-17, 1997.

3. "Coupled-Cluster Approach to Static Molecular Properties," "Coupled Cluster Theory and Electron Correlation" workshop, "Fifty Years of the Correlation Problem," Cedar Key, Florida, U.S.A., June 15-19, 1997, a satellite meeting of the 9th International Congress of Quantum Chemistry, Atlanta, Georgia, U.S.A., June 9-14, 1997.

4.* "Single-Reference Coupled-Cluster Methods for Quasi-Degenerate Electronic States," The symposium "Electronic Structure Theory: From Methods to Molecules and Materials," 100th Annual Meeting of the American Physical Society, Atlanta, Georgia, U.S.A., March 21-26, 1999.

5.* "Dynamics of Harpooning in van der Waals Molecules," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999.

6.* "Dynamics of Harpooning in van der Waals Molecules," "Vth International Conference on Molecular Spectroscopy," Lądek-Zdrój, Poland, September 26-30, 1999.

7.* "Method of Moments of Coupled-Cluster Equations: A New Approach to the Many-Electron Correlation Problem," The 2000 Florida Award Symposium (honoring Dr. Rodney J. Bartlett's work), FAME 2000 (Florida Annual Meeting and Exposition, organized by the Florida Section of the American Chemical Society), Orlando, Florida, U.S.A., May 12, 2000.

8.* "Dynamics of Photo-Induced Charge Transfer in van der Waals Molecules," Joint Polish-German Conference on Modern Optics: Fundamental Aspects of Spectroscopy and Environmental Applications, Jurata near Gdańsk, Poland, September 17-22, 2000.

9.* "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," the 41st Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 24-March 2, 2001.

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

10.* "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," First Southern School on Computational Chemistry (one of the two formal lectures), Orange Beach, Alabama, March 23-24, 2001.

11.* "Effect of the Potential Energy Surface on the Dynamics of Weakly Bound Precursor Complexes and New "Black-Blox" Coupled-Cluster Methods for Entire Potential Energy Surfaces of Reactive Molecular Systems," The symposium "First Principles Chemical Reaction Dynamics," 222nd American Chemical Society National Meeting, Chicago, Illinois, U.S.A., August 26-30, 2001.

12.* "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," 34th Midwest Theoretical Chemistry Conference, University of Minnesota, Minneapolis, Minnesota, U.S.A., October 5-6, 2001.

13.** "Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Quasi-Degenerate Ground States, Molecular Potential Energy Surfaces, and Excited States," Institute for Nuclear Theory workshop on "Advanced Computational Methods for Solving the Nuclear Many-Body Problem," Seattle, Washington, U.S.A., March 12-15, 2002.

14.** "New Single- and Multi-Reference Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," The symposium "Recent Advances in Electron Correlation Methodology," 223rd American Chemical Society National Meeting, Orlando, Florida, U.S.A., April 7-11, 2002.

15.** "Method of Moments of Coupled-Cluster Equations: A New Framework for Designing Accurate Electronic Structure Methods," Fourth International Congress of the International Society for Theoretical Chemical Physics (ICTCP-IV), Marly-le-Roi near Paris, France, July 9-16, 2002 [invited plenary lecture].

16.** "Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing Highly Accurate Electronic Structure Methods," International Symposium on Frontiers in Molecular Science 2002, Qingdao, China, July 15-18, 2002.

17.** "Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," 6th World Congress of Theoretically Oriented Chemists (WATOC02), Lugano, Switzerland, August 4-9, 2002 [invited contributed talk].

18.** "Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing Highly Accurate (Virtually Exact) and Inexpensive Electronic Structure Methods," 11th Conference on Current Trends in Computational Chemistry, Jackson, Missisipi, U.S.A., November 1-2, 2002.

19.** "New Alternatives for Accurate Electronic Structure Calculations of Molecular Potential Energy Surfaces," The symposium "New Electronic Structure Methods: From Molecules to Materials," 225th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., March 23-27, 2003.

20.** "Single- and Multi-reference Coupled-Cluster Methods for Quasidegenerate Electronic States and Bond Breaking," The symposium "Bond-Breaking Methods in Gas and Condensed Phases," 226th American Chemical Society National Meeting, New York, New York, U.S.A., September 7-11, 2003.

21.** "Noniterative Coupled-Cluster Methods for Accurate Calculations of Excited Electronic States," The symposium "The Systematic Treatment of Electron Correlation. A Celebration of the Science of Rodney J. Bartlett," St. Simons Island, Georgia, U.S.A., April 23-25, 2004.

22.** "Coupled-Cluster Method: An Accurate Ab Initio Theory of Atoms, Molecules, Nuclei, and Other Many-Fermion Systems," International Workshop on Microscopic Approaches to Nuclear Structure Calculations," UMIST, Manchester, U.K., July 4-8, 2004.

23.** "Coupled-Cluster Approaches to Atoms, Molecules, and Nuclei," Workshop "New Perspectives on p-Shell Nuclei," Michigan State University, East Lansing, Michigan, U.S.A., July 22-24, 2004.

24.** "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States," International conference "Molecular Quantum Mechanics: the No Nonsense Path to Progress" honoring Professor Nicholas Handy's work, St. John's College, Cambridge University, Cambridge, U.K., July 24-29, 2004.

25.** "Renormalized Coupled-Cluster Methods and their Automated Parallel Computer Implementation with Tensor Contraction Engine," The symposium "Symbolic Calculation in Chemistry," 228th American Chemical Society National Meeting, Philadelphia, Pennsylvania, U.S.A., August 22-26, 2004.

26.** "Coupled Cluster Calculations of Ground and Excited States of Nuclei," International Conference on Exotic Nuclei and Atomic Masses, ENAM-04, Pine Mountain, Georgia, U.S.A., September 12-16, 2004.

27.** "Non-Iterative Coupled-Cluster Methods For Accurate Calculations of Excited Electronic States," Ninth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-IX, Les Houches, Grenoble, France, September 25-30, 2004.

28.** "Coupled Cluster Calculations of Ground and Excited States of Nuclei," Ninth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-IX, Les Houches, Grenoble, France, September 25-30, 2004.

29.** "Coupled-Cluster Approaches to Atoms, Molecules, and Nuclei," Institute for Nuclear Theory workshop "Microscopic Nuclear Structure Theory," "Nuclear Forces and the Quantum Many-Body Problem," Seattle, Washington, U.S.A., October 4-8, 2004.

30.** "Coupled-Cluster Method: Highly Accurate Microscopic Approach to Molecular Systems and Nuclei," Workshop "Nuclei and Mesoscopic Physics," Michigan State University, East Lansing, Michigan, U.S.A., October 23-26, 2004.

31.** "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States," 7th World Congress of Theoretically Oriented Chemists (WATOC05), Cape Town, South Africa, January 16-21, 2005.

32.** "Renormalized and Active-Space Coupled-Cluster Methods: Two Approaches to Electronic Quasi-Degeneracies and Open-Shell Problems," Fifth Congress of the International Society for Theoretical Chemical Physics (ICTCP-V), New Orleans, Louisiana, U.S.A., July 20-26, 2005 [invited plenary lecture].

33.** "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States," The symposium "Theoretical Determination of Energy Landscapes: Methodology and Applications," 230th American Chemical Society National Meeting, Washington, DC, U.S.A., August 28 - September 1, 2005.

34.** "Renormalized and Active-Space Coupled-Cluster Methods: Two Approaches to Quasi-Degeneracies and Open-Shell Problems," Conference on Microscopic Approaches to Many-Body Theory, in honor of Professor Raymond Bishop, The University of Manchester, Manchester, U.K., August 31 - September 3, 2005.

35.** "Active-Space Coupled-Cluster Method: An Inexpensive and Highly Accurate Approach to Electronic Quasi-Degeneracies and Open-Shell Problems," Tenth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-X, Carthage, Tunisia, September 1-7, 2005.

36.** "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [invited plenary lecture].

37.** "Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Bond Breaking and Electronic Excitations in Molecules to Properties of Atomic Nuclei," The Centro Internacional de Matemática Workshop "Mathematics in Chemistry," Lisbon, Portugal, July 19-21, 2006.

38.** "Advances in Electronic Structure Theory: Single-Reference Coupled-Cluster Methods for Multi-Reference Problems," Sixth Canadian Computational Chemistry Conference (CCCC6), Vancouver, British Columbia, Canada, July 26-30, 2006 [invited plenary lecture].

39.** "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," Eleventh European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XI, St. Petersburg, Russia, August 20-25, 2006.

40.** "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," International Conference "Recent Trends in Many-Body Methods for Electronic Structure and Properties of Atoms and Molecules," Bhubaneswar and Puri, Orissa, India, January 11-13, 2007.

41.** "Active-Space Coupled-Cluster Methods for Bond Breaking, Excited Electronic States, and Open-Shell Systems," International Conference "Practicing Chemistry with Theoretical Tools, on the Occasion of Professor Mark S. Gordon's 65th Birthday," Kihei, Hawaii, U.S.A., January 15-18, 2007.

42.** "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," 39th Midwest Theoretical Chemistry Conference, Indiana University, Bloomington, Indiana, U.S.A., June 28-30, 2007.

43.** "Coupled-Cluster Theory: An Overview of the Basic Formalism and Applications to Molecular and Nuclear Structure Problems," Workshop on Advanced Many-body Methods for Nuclear Structure European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Trento, Italy, July 2-6, 2007.

44.** "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Applications to Radicals, Biradicals, and Bond Breaking," Twelfth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XII, London, U.K., August 30 - September 5, 2007.

45.** "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Applications to Radicals, Biradicals, Reaction Pathways, and Photochemistry," "IXth International Conference on Molecular Spectroscopy: From Molecules to Molecular Biological Systems and Molecular Materials: Role of Molecular Interactions and Recognition," Wrocław – Lądek-Zdrój, Poland, September 12-16, 2007.

46.** "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell Systems," The symposium "Electronic Structure and Reaction Dynamics of Open-shell Species," 235th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., April 6-10, 2008.

47.** "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," Sixth Congress of the International Society for Theoretical Chemical Physics (ICTCP-VI), Vancouver, British Columbia, Canada, July 19-24, 2008 [invited plenary lecture].

48.** "Coupled-Cluster Theory: A Brief Overview of Modern Methods and Applications to Nuclear Structure," the WE-Heraeus-Seminar "Ab-Initio Nuclear Structure - Where do we stand?", Bad Honnef, Germany, July 28-30, 2008.

49.** "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2008), Sydney, Australia, September 14-19, 2008.

50.** "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," The International Conference "Theory and Applications of Computational Chemistry 2008 (TACC 2008)," Shanghai, China, September 23-27, 2008 [invited plenary lecture].

51.** "Extending Electronic Structure Theory to Complex Molecular Problems: Local Correlation Coupled-Cluster and Correlation Energy Scaling Methodologies," The symposium "Advances in Electronic Structure Theory and First Principles Dynamics," 237th American Chemical Society National Meeting, Salt Lake City, Utah, U.S.A., March 22-26, 2009.

52.** "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States," 30th Annual Combustion Research Meeting, Airlie Conference Center, Warrenton, Virginia, U.S.A., May 26-29, 2009.

53.** "Coupled-Cluster Theory: From Quantum Chemistry to Applications in Nuclear Physics," International Workshop "Linking Nuclei, Molecules, and Condensed Matter: Computational Quantum Many-Body Approaches," European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Trento, Italy, July 6-10, 2009.

54.** "Dealing with Strong Electron Correlations in Quantum Chemistry via Renormalized, Active-Space, and Multi-Reference Coupled-Cluster Methods," The symposium "New Developments in Strongly Correlated Electrons," 238th American Chemical Society National Meeting, Washington, DC, U.S.A., August 16-20, 2009.

55.** "Extending Electronic Structure Theory to Complex Molecular Problems: Local Correlation Coupled-Cluster and Correlation Energy Scaling Methodologies," Fourteenth International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XIV, San Lorenzo de El Escorial, Madrid, Spain, September 13-19, 2009.

56.** "Dealing with Strong Electron Correlations in Quantum Chemistry via Renormalized, Active Space, and Multireference Coupled-Cluster Methods," An International Symposium "Recent Advances in Many Electron Theories," Shankarpur, West Bengal, India, January 5-7, 2010.

57.** "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," the 50th Sanibel Symposium, St. Simons Island, Georgia, U.S.A., February 24-March 2, 2010.

58.** "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," International conference "Molecular Quantum Mechanics: From Methylene to DNA and Beyond" honoring Professor Henry F. Schaefer's work, University of California at Berkeley, Berkeley, California, May 24-29, 2010.

59.** "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," 17th Canadian Symposium on Theoretical Chemistry, Edmonton, Alberta, Canada, July 25-30, 2010.

60.** "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," Fifteenth International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XV, Magdalene College, Cambridge University, Cambridge, U.K., August 31 - September 5, 2010.

61.** "Dealing with Chemical Reaction Pathways and Electronic Excitations in Molecular Systems via Renormalized and Active-Space Coupled-Cluster Methods," 18th European Conference on Dynamics of Molecular Systems, MOLEC XVIII, Curia, Portugal, September 5-10, 2010.

62.** "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," 9th Central European Symposium on Theoretical Chemistry, CESTC 2010, Nový Smokovec, Slovakia, September 12-15, 2010.

63.** "Dealing with Chemical Reaction Pathways and Electronic Excitations in Molecular Systems via Renormalized and Active-Space Coupled-Cluster Methods," 8th International Conference of Computational Methods in Sciences and Engineering (ICCMSE

2010), symposium "Methods in Quantum Chemistry" in honor of Jiri Čížek and Josef Paldus, Kos, Greece, October 3-8, 2010 [invited featured lecture].

64.** "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," The symposium "Fragment and Local Orbital Methods in Electronic Structure Theory," 241st American Chemical Society National Meeting, Anaheim, California, U.S.A., March 27-31, 2011.

65.** "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," 11th Annual CERMM Symposium, Centre for Research in Molecular Modeling, Concordia University, Montreal, Canada, June 4-5, 2011 [invited keynote lecture].

66.** "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," 94th Canadian Chemistry Conference and Exhibition, General Physical, Theoretical, and Computational Chemistry Session, Montreal, Canada, June 5-9, 2011.

67.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems and their Multi-Level Generalizations," Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2011), Santiago de Compostela, Spain, July 17-22, 2011.

68.** "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," WATOC 2011 Satellite Conference "Strongly Correlated Systems, Cooperativity, and Valence-Bond Theory," A Coruña, Spain, July 23-24, 2011.

69.** "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," The symposium "Reduced Density Matrices in Quantum Chemistry," 242nd American Chemical Society National Meeting, Denver, Colorado, U.S.A., August 28 - September 1, 2011.

70.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems and their Multi-Level Generalizations," The symposium "Quantum Chemistry: Methodology," 242nd American Chemical Society National Meeting, Denver, Colorado, U.S.A., August 28 - September 1, 2011.

71.** "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," The symposium "Quantum Chemistry: DFT," 242nd American Chemical Society National Meeting, Denver, Colorado, U.S.A., August 28 - September 1, 2011.

72.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems and their Multi-Level Generalizations," Seventh Congress of the International Society for Theoretical Chemical Physics (ICTCP-VII), Tokyo, Japan, September 2-8, 2011.

73.** "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," XVI-th International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XVI, Kanazawa, Japan, September 11-17, 2011.

74.** "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," An International Symposium "Recent Advances in Many Electron Theories II, 2011," Puri, Orissa, India, December 1-4, 2011.

75.** "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," The Fifth Asian Pacific Conference of Theoretical and Computational Chemistry (APCTCC 2011), Rotorua, New Zealand, December 9-13, 2011.

76.** "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States (Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods)," 33rd Annual Combustion Research Meeting, Bolger Center, Potomac, Maryland, U.S.A., May 29 - June 1, 2012.

77.** "Recent Progress in Renormalized and Active-Space Coupled-Cluster Methods," The symposium "Coupled-Cluster Theory and Related Methods," A Satellite Symposium to the 14th International Congress of Quantum Chemistry, Boulder, Colorado, U.S.A., July 1-3, 2012.

78.** "Multi-level Extensions of the Cluster-in-Molecule Local Correlation Methodology Aimed at Chemical Reaction Pathways Involving Large Molecular Systems," The symposium "Bridging the Gap between Ab Initio and Classical Simulations," 244th American Chemical Society National Meeting, Philadelphia, Pennsylvania, U.S.A., August 19-23, 2012.

79.** "Combining Active-Space Coupled-Cluster Methods with Moment Energy Corrections via the CC($P;Q$) Methodology, with Benchmark Calculations for Bond Breaking and Biradical Transition States," The symposium "Exploring Potential Energy Surfaces in Quantum Chemistry: A Tribute to H. Bernhard Schlegel," 244th American Chemical Society National Meeting, Philadelphia, Pennsylvania, U.S.A., August 19-23, 2012.

80.** "Accurate Characterization of Reaction Pathways Relevant to Combustion and Electronic Excitations in Radicals and Biradicals via Renormalized and Active-Space Coupled-Cluster Theories, their Merger, and Open-Shell Extensions," The symposium on Combustion Chemistry, 245th American Chemical Society National Meeting, New Orleans, Lousiana, U.S.A., April 7-11, 2013.

81.** "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," The symposium "Quantum Chemistry: Methodology," 245th American Chemical Society National Meeting, New Orleans, Lousiana, U.S.A., April 7-11, 2013.

82.** "The Cobalt-Methyl Dissociation and Electronic Transitions in Methylcobalamin: Insights from the Coupled-cluster, Multireference Perturbation Theory, and Density Functional Theory Calculations," The symposium "Bioinorganic Chemistry: Proteins and Enzymes and Model Systems," 245th American Chemical Society National Meeting, New Orleans, Lousiana, U.S.A., April 7-11, 2013.

83.** "Recent Progress in the Active-Space Electron-Attached and Ionized Equation-of-Motion Coupled-Cluster Methodologies," 7th International Conference "Molecular Quantum Mechanics" entitled "Electron Correlation: The Many-Body Problem at the Heart of Chemistry," in honor of Professor Rodney J. Bartlett, Lugano, Switzerland, June 2-7, 2013.

84.** "Recent Progress in the Active-Space Electron-Attached and Ionized Equation-of-Motion Coupled-Cluster Methodologies," Eighth Congress of the International Society for Theoretical Chemical Physics (ISTCP-VIII), Budapest, Hungary, August 25-31, 2013.

85.** "Single-Reference Coupled-Cluster Methods for Multi-Reference Molecular Problems," 6th Conference "Current Trends in Theoretical Chemistry" (CTTC VI), Cracow, Poland, September 1-5, 2013.

86.** "Understanding Photochemistry and Photo-ionization Dynamics with Highly Correlated Electronic Structure Methods: Two Examples that Highlight the Transformative Role of Theory in the Interpretation of Experimental Observations," XVIII-th International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XVIII), Paraty (Rio de Janeiro), Brazil, December 1-7, 2013.

87.** "Understanding Photochemistry and Photo-ionization Dynamics with Highly Correlated Electronic Structure Methods: Two Examples that Highlight the Transformative Role of Theory in the Interpretation of Experimental Observations," The symposium "A Little Insight Goes a Long Way," 247th American Chemical Society National Meeting, Dallas, Texas, U.S.A., March 16-20, 2014.

88.** "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(P;Q) Methodology: Connected Triple and Quadruple Excitations," The symposium "Quantum Chemistry: Methodology," 247th American Chemical Society National Meeting, Dallas, Texas, U.S.A., March 16-20, 2014.

89.** "Utility of New Generations of Coupled-Cluster Methods and Algorithms in Catalytic and Structural Properties of Gold Nanoparticles," The symposium "Quantum Chemistry: Applications," 247th American Chemical Society National Meeting, Dallas, Texas, U.S.A., March 16-20, 2014.

90.** "Single-Reference Coupled-Cluster Methods for Multi-Reference Molecular Problems," Nordita program on "Computational Challenges in Nuclear and Many-Body Physics," Stockholm, Sweden, September 15 - October 10, 2014.

91.** "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(P;Q) Methodology," Tenth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2014), Santiago, Chile, October 5-10, 2014.

92.** "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(P;Q) Methodology," The Fourteenth Theoretical Chemistry Symposium (TCS 2014), Pune, India, December 18-21, 2014 [invited keynote lecture].

93.** "Understanding Photochemistry and Photoelectron Spectra with Highly Correlated Electronic Structure Methods Based on Coupled-Cluster Theory," The symposium "Modeling Excited States of Complex Systems," 249th American Chemical Society National Meeting, Denver, Colorado, U.S.A., March 22-26, 2015.

94.** "Aerobic Oxidation of Methanol to Formic Acid on Au_8^-: Benchmark Analysis Based on Completely Renormalized Coupled-Cluster and Density Functional Theory Calculations," The symposium "Computational Chemical Dynamics: Advancing Our Understanding of Chemical Processes in Gas-Phase, Biomolecular and Condensed-Phase Systems," 249th American Chemical Society National Meeting, Denver, Colorado, U.S.A., March 22-26, 2015.

95.** "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(P;Q) Methodology: Ground and Excited States," The symposium "Quantum Chemistry: Methodology," 249th American Chemical Society National Meeting, Denver, Colorado, U.S.A., March 22-26, 2015.

96.** "Molecular Systems from the Equation-of-Motion Coupled-Cluster Theory" or "Understanding Electronic Excitation, Multi-Photon Ionization, and Photo-Electron Spectra with the Equation-of-Motion Coupled-Cluster Theory," Workshop of the Espace de Structure Nucléaire Théorique on "Near-Degenerate Systems in Nuclear Structure and Quantum Chemistry from Ab-Initio Many-Body Methods," CEA Saclay, France, March 30 - April 2, 2015.

97.** "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems," The symposium "Recent Advances in Electronic Structure Theory (RAEST2015)," A Satellite Symposium to the 15th International Congress of Quantum Chemistry, Nanjing, China, June 1-6, 2015.

98.** "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Theories for High-Accuracy *Ab Initio* Computations of Chemical Reaction Profiles Involving Biradical Transition States and Electronic Spectra of Radical and Polyradical Species," The symposium "From Diradicals and Polyradicals to Functionalized Materials: Theory Meets Experiment," 250th American Chemical Society National Meeting, Boston, Massachusetts, U.S.A., August 16-20, 2015.

99.** "Utility of New Generations of Coupled-Cluster Methods and Algorithms in Catalytic, Structural, and Optical Properties of Gold Nanoparticles," The symposium "Interplay between Theory and Experiment in Catalytic Research," the 2015 International Chemical Congress of Pacific Basin Societies (Pacifichem 2015), Honolulu, Hawaii, U.S.A., December 15-20, 2015.

100.** "Coupled-Cluster Interpretation of the Photoelectron Spectra of Ag_3^- and Au_3^-," 26th Austin Symposium on Molecular Structure and Dynamics, Dallas, Texas, U.S.A., March 5-7, 2016.

101.** "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States (Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: CC(P;Q) Formalism)," 2nd Computational and Theoretical Chemistry Research PI Meeting, Gaithersburg, Maryland, U.S.A., May 15-18, 2016.

102.** "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems," TSRC Workshop "Low-Scaling and Unconventional Electronic Structure Techniques" (LUEST 2016), 3rd edition, Telluride, Colorado, U.S.A., June 1-5, 2016.

103.** "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: CC(P;Q) Formalism," Ninth Congress of the International Society for Theoretical Chemical Physics (ISTCP-IX), Grand Forks, North Dakota, U.S.A., July 17-22, 2016.

104.** "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: CC(P;Q) Formalism," The International Conference "Theory and Applications of Computational Chemistry 2016 (TACC 2016)," Seattle, Washington, August 28 - September 2, 2016.

105.** "Understanding Photochemistry and Photoelectron Spectra with Highly Correlated Electronic Structure Methods based on Coupled-Cluster Theory," 7th Conference "Current Trends in Theoretical Chemistry" (CTTC VII), Cracow, Poland, September 4-8, 2016.

106.** "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," EMN Meeting on Computation and Theory (Energy, Materials, and Nanotechnology), workshop "Novel Electron Correlation Methods for Complex Systems," Las Vegas, Nevada, U.S.A., October 10-14, 2016.

107.** "Coupled-Cluster Interpretation of the Photoelectron Spectra of Ag_3^- and Au_3^-," GAMESS*7557*SSEMAG Palindromic Birthday Theory Symposium, on the Occasion of Professor Mark S. Gordon's 75th and Professor Kim K. Baldridge 57th Birthdays," Lihue, Hawaii, U.S.A., January 16-18, 2017.

108.** "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," An International Conference "Recent Advances in Many-Electron Theory (RAMET-2017)," Goa, India, February 9-12, 2017.

109.** "The 1966 *Journal of Chemical Physics* Article by Jiří Čížek: What Is in It and Why Is It so Important," the 57th Sanibel Symposium, a special symposium recognizing the 50th Anniversary of Jiří Čížek's 1966 Paper on Coupled-Cluster Theory, St. Simons Island, Georgia, U.S.A., February 19-24, 2017.

110.** "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: CC(P;Q) Formalism," The symposium "Electronic Structure of Complex Chemical Systems," 254th American Chemical Society National Meeting, Washington, DC, U.S.A., August 20-24, 2017.

111.** "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," PHYS Awards Symposium, 254th American Chemical Society National Meeting, Washington, DC, U.S.A., August 20-24, 2017.

112.** "Stochastic CC(P;Q) Theory: Converging High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," Eleventh Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2017), Munich, Germany, August 27 - September 1, 2017.

113.** "High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," 15th Central European Symposium on Theoretical Chemistry, CESTC 2017, Wisła, Poland, September 3-6, 2017.

114.** "High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," 27th Austin Symposium on Molecular Structure and Dynamics, Dallas, Texas, U.S.A., March 3-5, 2018.

115.** "Introduction to Single-Reference Many-Body Perturbation Theory and its Diagrammatic Representation," Workshop of the Espace de Structure Nucléaire Théorique on "Many-Body Perturbation Theories in Modern Quantum Chemistry and Nuclear Physics," CEA Saclay, France, March 26-30, 2018.

116.** "Perturbative Corrections to Non-perturbative Methods" or "High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," Workshop of the Espace de Structure Nucléaire Théorique on "Many-Body Perturbation Theories in Modern Quantum Chemistry and Nuclear Physics," CEA Saclay, France, March 26-30, 2018.

117.** "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," 4th Computational and Theoretical Chemistry Research PI Meeting, Gaithersburg, Maryland, U.S.A., May 21-24, 2018.

118.** "High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," TSRC Workshop "Low-Scaling and Unconventional Electronic Structure Techniques" (LUEST 2018), 4th edition, Telluride, Colorado, U.S.A., June 4-8, 2018.

119.** "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," The joint Annual Workshop on Recent Developments in Electronic Structure Methods (ES18) and Penn Conference in Theoretical Chemistry (PCTC18), Philadelphia, Pennsylvania, U.S.A., June 10-14, 2018.

120.** "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," The symposium "Strong Correlation in Electronic Structure Theory," A Satellite Symposium to the 16th International Congress of Quantum Chemistry, Strasbourg, France, June 24-27, 2018.

121.** "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," 28th Canadian Symposium on Theoretical and Computational Chemistry (CSTCC 2018), Windsor, Ontario, Canada, July 15-19, 2018.

122.** "Toward Exact Quantum Chemistry: Accurate Electronic Energies by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," The international conference "Quantum International Frontiers 2018," Changsha, Hunan Province, China, October 17-21, 2018 [invited Frontier Lecture].

123.** "Toward Exact Quantum Chemistry by Combining Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Mainz-Kobe Joint Workshop on "Solving the Full Configuration Interaction Problem," RIKEN Center for Computational Science, Kobe, Japan, November 26-27, 2018 [teleconference session].

124.** "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," TSRC Workshop "New Frontiers in Electron Correlation," 2nd edition, Telluride, Colorado, U.S.A., June 10-14, 2019.

125.** "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Tenth Congress of the International Society for Theoretical Chemical Physics (ISTCP-X), symposium entitled "Emergent Electronic Structure Methods," Tromsø, Norway, July 11-17, 2019.

126.** "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," 8th Conference "Current Trends in Theoretical Chemistry" (CTTC VIII), Cracow, Poland, September 1-4, 2019.

127.** "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," 20th International Conference on Recent Progress in Many-Body Theories, Toulouse, France, September 9-13, 2019.

128.** "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," The Utah Workshop on Quantum Methods in Molecular and Solid-State Theory, Park City, Utah, U.S.A., September 22-27, 2019.

129.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Workshop on New Methods for Strongly Correlated Electrons, Qingdao, China, October 9-13, 2019.

130.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," The international conference "Quantum International Frontiers 2019," Shanghai, China, November 18-22, 2019 [invited Frontier Lecture].

131.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," the 60th Sanibel Symposium, St. Simons Island, Georgia, U.S.A., February 16-21, 2020.

132.** "High-Accuracy Electronic Energetics by Stochastic and Deterministic Wave Function Sampling and Coupled-Cluster Computations," TSRC Workshop "Low-Scaling and Unconventional Electronic Structure Techniques" (LUEST 2020), 5th edition, Telluride, Colorado, U.S.A., June 1-5, 2020.
DUE TO COVID-19, REPLACED BY VIRTUAL WORKSHOP, June 1-5 and June 8-9, 2020 [lecture via Zoom].

133.** "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States (Toward Exact Quantum Chemistry)," 2020 Computational and Theoretical Chemistry Virtual Conference Series (July 16, July 30, August 13, 2020), Germantown, Maryland, U.S.A., August 13, 2020 [lecture via Zoom].

134.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," The Physical, Theoretical, and Computational Chemistry Virtual Seminar Series, Chemical Institute of Canada, December 1, 2020 [lecture via Zoom].

135.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," TSRC Workshop "New Frontiers in Electron Correlation," 3rd edition, Telluride, Colorado, U.S.A., June 14-18, 2021 [virtual workshop; lecture via Zoom].

136.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," The 4th TSRC Workshop "New Developments in Coupled-Cluster Theory," Telluride, Colorado, U.S.A., July 19-23, 2021 [hybrid format; lecture via Zoom].

137.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," International Symposium on Correlated Electrons (SymCorrel21), Munich Center for Quantum Science and Technology, Munich, Germany, October 5-7, 2021 [virtual workshop; lecture via Zoom].

138.** "Computational Studies of FR0-SB, a Novel Organic Compound that Deprotonates Alcohols upon Photoexcitation," International conference in the series "New Horizons in Scientific Software (NHISS 2021)" entitled "Light-Matter Interaction: Theory Meets Experiment," Jeju Island, South Korea, November 22-25, 2021 [hybrid format; lecture via Zoom].

139.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," The Seventeenth Theoretical Chemistry Symposium (TCS 2021), Indian Institute of Science Education and Research Kolkata, Mohanpur, Nadia, West Bengal, India, December 11-14, 2021 [virtual symposium; invited plenary lecture].

140.** "Externally Corrected Coupled-Cluster Methods Using Selected Configuration Interaction and FCIQMC," the 61st Sanibel Symposium, invited session on New Directions in CC Theory, St. Simons Island, Georgia, U.S.A., February 13-18, 2022 [in-person invited plenary lecture].

141.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," Chris Cramer 60th Birthday Symposium, 263rd American Chemical Society National Meeting, San Diego, California, U.S.A., March 20-24, 2022 [in-person and virtual meeting; pre-recorded virtual presentation].

142.** "Recent Advances in Externally Corrected Coupled-Cluster Methods," 10th International Conference "Molecular Quantum Mechanics" entitled "Molecular Quantum Mechanics: Innovation, Impact, and Insight," in honor of Professors Gustavo Scuseria and Martin Head-Gordon, Blacksburg, Virginia, U.S.A., June 26 - July 1, 2022 [invited plenary lecture].

143.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," Twelfth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2020), Vancouver, British Columbia, Canada, August 16-21, 2020.
DUE TO COVID-19, RESCHEDULED TO July 3-8, 2022.

144.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," The 2020 American Conference on Theoretical Chemistry (ACTC 2020), Palisades Tahoe (formerly Squaw Valley), California, U.S.A., July 26-30, 2020.
DUE TO COVID-19, RESCHEDULED TO July 24-28, 2022; renamed ACTC 2022.

145.** "Recent Advances in Externally Corrected Coupled-Cluster Methods," The symposium "Quantum Chemistry: Current and Future Frontiers," 264th American Chemical Society National Meeting, Chicago, Illinois, U.S.A., August 21-25, 2022 [in-person and virtual meeting; in-person talk].

146.** "Recent Advances in Externally Corrected Coupled-Cluster Methods," OPERA-2020 (Operators, Perturbations, Electrons, Relativity, and Multi-Scale Applications), an international symposium on theoretical chemistry in honour of Prof. Jürgen Gauss on the occasion of his 60th birthday, Ingelheim am Rhein, Germany, September 1-3, 2021.
DUE TO COVID-19, RESCHEDULED TO August 31 - September 2, 2022.

147.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Modeling and Design of Molecular Materials 2020 (MDMM 2020) Conference, Gdańsk, Poland, September 21-24, 2020.
DUE TO COVID-19, RESCHEDULED TO September 19-22, 2022; renamed MDMM 2022.

148.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," International conference in the series "New Horizons in Scientific Software (NHISS 2022)" entitled "The New Collaborative Platform Goes Life," Jeju Island, South Korea, December 12-15, 2022 [hybrid format; lecture via Zoom].

149.** "Computational Studies of FR0-SB, a Novel Organic Compound that Deprotonates Alcohols upon Photoexcitation," 28th Austin Symposium on Molecular Structure and Dynamics, Dallas, Texas, U.S.A., February 17-20, 2023.

150.** "Externally Corrected Coupled-Cluster Methods: Review and Recent Progress," The symposium "Strong Correlation in Molecules," A Satellite Symposium to the 17th International Congress of Quantum Chemistry, Znojmo, Czech Republic.
DUE TO COVID-19, RESCHEDULED TO June 20-23, 2023 [special invited lecture during the session dedicated to the memory of Josef Paldus].

151.** "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches," 17th International Congress of Quantum Chemistry, Bratislava, Slovakia, June 21-26, 2021.
DUE TO COVID-19, RESCHEDULED TO June 26 - July 1, 2023 [invited plenary lecture].

152.** "Computational Studies of FR0-SB, a Novel Organic Compound that Deprotonates Alcohols upon Photoexcitation," The 41st Midwest Undergraduate Computational Chemistry Consortium (MU3C) Conference, Michigan State University, East Lansing, Michigan, U.S.A., August 1-2, 2023.

153.** "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches," The 5th Conference on Theory and Applications of Computational Chemistry (TACC 2020), Sapporo, Japan, September 7-12, 2020.
DUE TO COVID-19, RESCHEDULED TO September 4-9, 2023; renamed TACC 2023.

154.** "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches," 26th International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XXVI), Jaipur, Rajasthan, India, October 14-20, 2023 [hybrid format; lecture via Zoom].

155.** "Recent Progress in Externally Corrected Coupled-Cluster Methods: Following the Footsteps of a Legend (Lecture in Memory of Professor Josef Paldus)," The 37th Symposium on Chemical Physics at the University of Waterloo, Waterloo, Ontario, Canada, November 3-5, 2023 [special invited lecture in memory of Josef Paldus].

156.** "Addressing Strong Correlations Using Approximate Coupled-Pair Ideas: Following the Footsteps of a Legend (Lecture in Memory of Professor Josef Paldus)," the 63rd Sanibel Symposium, invited session on Coupled-Cluster Theory, St. Augustine Beach, Florida, U.S.A., February 25 - March 1, 2024 [invited plenary lecture].

157.** "Remembering Professor Josef Paldus: Pioneer of Modern Electronic Structure Theory and Caring Mentor, Educator, and Friend," Symposium "Advances in Electronic Structure Theory: A Symposium in Honour of Joe Paldus," the 107th Canadian Chemistry Conference and Exhibition (CSC 2024), Winnipeg, Manitoba, Canada, June 2-6, 2024.

158.** "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches," 30th Canadian Symposium on Theoretical and Computational Chemistry (CSTCC 2024), Halifax, Nova Scotia, Canada, July 21-25, 2024.

159.** "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches," The 5th TSRC Workshop "New Developments in Coupled-Cluster Theory," Telluride, Colorado, U.S.A., July 29 - August 2, 2024.

160.** "Converging High-Level Coupled-Cluster Energetics with Semi-Stochastic, CIPSI-Driven, and Adaptive CC(P;Q) Methods," 9th Conference "Current Trends in Theoretical Chemistry" (CTTC IX), Cracow, Poland, September 1-5, 2024.

161.** "Converging High-Level Coupled-Cluster Energetics with Semi-Stochastic, CIPSI-Driven, and Adaptive CC(P;Q) Methods," Eleventh Congress of the International Society for Theoretical Chemical Physics (ISTCP-XI), symposium on Wave Function Theory for Electronic Structure, Qingdao, China, October 13-18, 2024.

162.** "Remembering Professor Josef Paldus: Pioneer of Modern Electronic Structure Theory and Caring Mentor, Educator, and Friend," Eleventh Congress of the International Society for Theoretical Chemical Physics (ISTCP-XI), Auqing Tang, Joe Paldus, and Bogumił Jeziorski Memorial Symposium and session on Chemical Insights, Qingdao, China, October 13-18, 2024.

163.** TBD, The symposium "Methods and Applications on Simulating Excited States: Molecular Dynamics, Spectroscopy, and Catalysis," 269th American Chemical Society National Meeting, San Diego, California, U.S.A., March 23-27, 2025.

164.** TBD, 11th Molecular Quantum Mechanics Conference (MQM 2025), in honor of Professors Hiroshi Nakatsuji and Kimihiko Hirao and in memory of Professors Keiji Morokuma and Shigeki Kato, Kyoto, Japan, May 23-28, 2025.

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

LIST OF ALL INVITED TALKS[†]

1. "Invariance Properties of the Multipole Expansion," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Warsaw, Poland, May 12, 1983.

2. "What Was Most Fascinating for Me in my Master of Science Research Project and will I Continue this Kind of Research in the Future," The Scientific Convention of the Polish Chemical Society and of the Association of Chemical Industry Engineers and Technicians, Katowice, Poland, September 22, 1983 [lecture on the occasion of receiving the Individual Prize of the Polish Chemical Society].

3. "Irreducible Tensor Operators in Theory of Long-Range Intermolecular Interactions," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Warsaw, Poland, April 5, 1984.

4. "Perturbation-Theoretical Description of Long-Range Intermolecular Interactions - the Application of Racah-Wigner Algebra and the Formalism of Irreducible Tensors," Nonlinear Optics Division, Institute of Physics, University of Poznań, Poland, March 29, 1988.

5. "Orthogonally Spin-Adapted Multi-Reference Coupled-Cluster Theory and Its Application to Model Systems with Varying Degree of Quasidegeneracy," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Warsaw, Poland, December 5, 1991.

6. "Application of the Hilbert-Space Coupled-Cluster Theory to Electronic States of the H_4 Model System," Workshop "Coupled Clusters in the Theory of Atoms and Molecules," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Warsaw, Poland, October 23-24, 1992.

7. "Recent Progress in Coupled Cluster Theory," Physical Chemistry Division Seminar, Department of Chemistry, University of Arizona, Tucson, Arizona, U.S.A., September 27, 1993.

8. "Recent Progress in Coupled Cluster Theory," Department of Chemistry, Indiana University, Bloomington, Indiana, U.S.A., January 3, 1994.

9. "Linear Response Coupled-Cluster Approach to Static Molecular Properties," The symposium "Frontiers in Electronic Structure Theory," 213th American Chemical Society National Meeting, San Francisco, California, U.S.A., April 13-17, 1997 [co-authors: A.E. Kondo, J. Paldus, and V. Špirko].

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

10. "Electron Correlation in Chemical Bonding," Department of Chemistry, York University, North York, Ontario, Canada, March, 1996.

11. "Coupled-Cluster Approach to Static Molecular Properties," "Coupled Cluster Theory and Electron Correlation" workshop, "Fifty Years of the Correlation Problem," Cedar Key, Florida, U.S.A., June 15-19, 1997, a satellite meeting of the 9th International Congress of Quantum Chemistry, Atlanta, Georgia, U.S.A., June 9-14, 1997.

12. "Electron Correlation in Molecules," Special Physical Chemistry Seminar, Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., August 14, 1997.

13. "Dynamics of Harpooning in van der Waals Molecules," Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., December 16, 1997.

14. "Dynamics of Harpooning in van der Waals Molecules," Quantum Theory Project Seminar, Quantum Theory Project, University of Florida, Gainesville, Florida, U.S.A., March 18, 1998.

15.* "Single-Reference Coupled-Cluster Methods for Quasi-Degenerate Electronic States," The symposium "Electronic Structure Theory: From Methods to Molecules and Materials," 100th Annual Meeting of the American Physical Society, Atlanta, Georgia, U.S.A., March 21-26, 1999.

16.* "Coupled-Cluster Theory: A Powerful Approach to Many-Electron Correlation Problem," Departmental Seminar, Department of Chemistry, University of Minnesota, Minneapolis, Minnesota, U.S.A., April 26, 1999.

17.* "Dynamics of Harpooning in van der Waals Molecules," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999.

18.* "Dynamics of Harpooning in van der Waals Molecules," "Vth International Conference on Molecular Spectroscopy," Lądek-Zdrój, Poland, September 26-30, 1999.

19.* "Method of Moments of Coupled-Cluster Equations: A New Approach to the Many-Electron Correlation Problem," Quantum Theory Seminar, Department of Applied Mathematics, University of Waterloo, Waterloo, Ontario, Canada, May 4, 2000.

20.* "Dynamics of Photo-Induced Charge Transfer in van der Waals Molecules," Chemical Physics Research Seminar, Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada, May 5, 2000.

21.* "Method of Moments of Coupled-Cluster Equations: A New Approach to the Many-Electron Correlation Problem," The 2000 Florida Award Symposium (honoring Dr. Rodney J. Bartlett's work), FAME 2000 (Florida Annual Meeting and Exposition, organized by the Florida Section of the American Chemical Society), Orlando, Florida, U.S.A., May 12, 2000.

22.* "Dynamics of Photo-Induced Charge Transfer in van der Waals Molecules," Joint Polish-German Conference on Modern Optics: Fundamental Aspects of Spectroscopy and Environmental Applications, Jurata near Gdańsk, Poland, September 17-22, 2000.

23.* "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Warsaw, Poland, September 29, 2000.

24.* "Dynamics of Photo-Induced Charge Transfer in van der Waals Molecules," Department of Chemistry, University of Arizona, Tucson, Arizona, U.S.A., October 23, 2000.

25.* "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," the 41st Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 24-March 2, 2001.

26.* "Dynamics of Photo-Induced Charge Transfer in van der Waals Molecules," Department of Chemistry and Computational Center for Molecular Structure and Interactions, Distinguished Lecture Series in Computational Chemistry and Physics, Jackson State University, Jackson, Missisipi, U.S.A., March 23, 2001.

27.* "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," First Southern School on Computational Chemistry (one of the two formal lectures), Orange Beach, Alabama, March 23-24, 2001.

28.* "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," NSCL Theory Journal Club, National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Michigan, U.S.A., June 22 and 26, 2001.

29.* "Effect of the Potential Energy Surface on the Dynamics of Weakly Bound Precursor Complexes and New "Black-Blox" Coupled-Cluster Methods for Entire Potential Energy Surfaces of Reactive Molecular Systems," The symposium "First Principles Chemical Reaction Dynamics," 222nd American Chemical Society National Meeting, Chicago, Illinois, U.S.A., August 26-30, 2001.

30.* "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," 34th Midwest Theoretical Chemistry Conference, University of Minnesota, Minneapolis, Minnesota, U.S.A., October 5-6, 2001.

31.* "Dynamics of Photo-Induced Charge Transfer in van der Waals Molecules," Institute of Physical and Theoretical Chemistry, Faculty of Chemistry, Wrocław University of Technology, Wrocław, Poland, October 19, 2001.

32.* "Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic, October 26, 2001.

33.** "Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," Faculty of Chemistry, University of Wrocław, Wrocław, Poland, November 9, 2001.

34.** "Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," Condensed Matter Physics Seminar, Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan, U.S.A., November 29, 2001.

35.** "Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," Department of Chemistry, Iowa State University, Ames, Iowa, U.S.A., March 6, 2002.

36.** "Advances in Electronic Structure Theory: Multi-Reference Coupled-Cluster Methods," Scalable Computing Laboratory, Ames Laboratory, USDOE, Iowa State University, Ames, Iowa, U.S.A., March 7, 2002.

37.** "Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Quasi-Degenerate Ground States, Molecular Potential Energy Surfaces, and Excited States," Institute for Nuclear Theory workshop on "Advanced Computational Methods for Solving the Nuclear Many-Body Problem," Seattle, Washington, U.S.A., March 12-15, 2002.

38.** "New Single- and Multi-Reference Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," The symposium "Recent Advances in Electron Correlation Methodology," 223rd American Chemical Society National Meeting, Orlando, Florida, U.S.A., April 7-11, 2002.

39.** "Method of Moments of Coupled-Cluster Equations: A New Framework for Designing Accurate Electronic Structure Methods," Fourth International Congress of the International Society for Theoretical Chemical Physics (ICTCP-IV), Marly-le-Roi near Paris, France, July 9-16, 2002 [invited plenary lecture].

40.** "Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing Highly Accurate Electronic Structure Methods," International Symposium on Frontiers in Molecular Science 2002, Qingdao, China, July 15-18, 2002.

41.** "Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," 6th World Congress of Theoretically Oriented Chemists (WATOC02), Lugano, Switzerland, August 4-9, 2002 [invited contributed talk].

42.** "Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing Highly Accurate (Virtually Exact) and Inexpensive Electronic Structure Methods," 11th Conference on Current Trends in Computational Chemistry, Jackson, Missisipi, U.S.A., November 1-2, 2002.

43.** "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited Electronic States," Lawrence Livermore National Laboratory, Livermore, California, U.S.A., November 13, 2002.

44.** "New Ideas in Electronic Structure Theory: Method of Moments of Coupled-Cluster Equations," Department of Chemistry, University of California at Berkeley, Berkeley, California, U.S.A., November 15, 2002.

45.** "New Ideas in Electronic Structure Theory: Method of Moments of Coupled-Cluster Equations," Department of Chemistry, University of North Dakota, Grand Forks, North Dakota, U.S.A., November 21, 2002.

46.** "New Ideas in Electronic Structure Theory: Method of Moments of Coupled-Cluster Equations," Department of Chemistry, North Dakota State University, Fargo, North Dakota, U.S.A., November 22, 2002.

47.** "New Alternatives for Accurate Electronic Structure Calculations of Molecular Potential Energy Surfaces," Department of Chemistry, Ohio State University, Columbus, Ohio, U.S.A., December 5, 2002.

48.** "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited Electronic States," National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Michigan, U.S.A., March 20, 2003.

49.** "New Alternatives for Accurate Electronic Structure Calculations of Molecular Potential Energy Surfaces," The symposium "New Electronic Structure Methods: From Molecules to Materials," 225th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., March 23-27, 2003.

50.** "Single- and Multi-reference Coupled-Cluster Methods for Quasidegenerate Electronic States and Bond Breaking," The symposium "Bond-Breaking Methods in Gas and Condensed Phases," 226th American Chemical Society National Meeting, New York, New York, U.S.A., September 7-11, 2003.

51.** "New Alternatives for Accurate Electronic Structure Calculations for Molecular Systems," Department of Chemistry and Biochemistry, Southern Illinois University at Carbondale, Carbondale, Illinois, U.S.A., October 3, 2003.

52.** "New Alternatives for Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems," Department of Physics, Central Michigan University, Mount Pleasant, Michigan, U.S.A., March 18, 2004.

53.** "Noniterative Coupled-Cluster Methods for Accurate Calculations of Excited Electronic States," The symposium "The Systematic Treatment of Electron Correlation. A Celebration of the Science of Rodney J. Bartlett," St. Simons Island, Georgia, U.S.A., April 23-25, 2004.

54.** "Coupled-Cluster Method: An Accurate Ab Initio Theory of Atoms, Molecules, Nuclei, and Other Many-Fermion Systems," International Workshop on Microscopic Approaches to Nuclear Structure Calculations," UMIST, Manchester, U.K., July 4-8, 2004.

55.** "Coupled-Cluster Approaches to Atoms, Molecules, and Nuclei," Workshop "New Perspectives on p-Shell Nuclei," Michigan State University, East Lansing, Michigan, U.S.A., July 22-24, 2004.

56.** "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States," International conference "Molecular Quantum Mechanics: the No Nonsense Path to Progress" honoring Professor Nicholas Handy's work, St. John's College, Cambridge University, Cambridge, U.K., July 24-29, 2004.

57.** "Renormalized Coupled-Cluster Methods and their Automated Parallel Computer Implementation with Tensor Contraction Engine," The symposium "Symbolic Calculation in Chemistry," 228th American Chemical Society National Meeting, Philadelphia, Pennsylvania, U.S.A., August 22-26, 2004.

58.** "Coupled Cluster Calculations of Ground and Excited States of Nuclei," International Conference on Exotic Nuclei and Atomic Masses, ENAM-04, Pine Mountain, Georgia, U.S.A., September 12-16, 2004.

59.** "Non-Iterative Coupled-Cluster Methods For Accurate Calculations of Excited Electronic States," Ninth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-IX, Les Houches, Grenoble, France, September 25-30, 2004.

60.** "Coupled Cluster Calculations of Ground and Excited States of Nuclei," Ninth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-IX, Les Houches, Grenoble, France, September 25-30, 2004.

61.** "Coupled-Cluster Approaches to Atoms, Molecules, and Nuclei," Institute for Nuclear Theory workshop "Microscopic Nuclear Structure Theory," "Nuclear Forces and the Quantum Many-Body Problem," Seattle, Washington, U.S.A., October 4-8, 2004.

62.** "New Alternatives for Accurate Quantum Calculations for Molecular Systems: Bond Breaking, Diradicals, and Excited Electronic States," Department of Physical Chemistry, University of Geneva, Switzerland, October 15, 2004.

63.** "Coupled-Cluster Method: Highly Accurate Microscopic Approach to Molecular Systems and Nuclei," Workshop "Nuclei and Mesoscopic Physics," Michigan State University, East Lansing, Michigan, U.S.A., October 23-26, 2004.

64.** "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States," 7th World Congress of Theoretically Oriented Chemists (WATOC05), Cape Town, South Africa, January 16-21, 2005.

65.** "New Alternatives for Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Bond Breaking and Diradicals to Excited Electronic States in Molecules and Atomic Nuclei," Department of Chemistry, Wayne State University, Detroit, Michigan, U.S.A., March 9, 2005.

66.** "New Alternatives for Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Bond Breaking and Diradicals to Excited Electronic States in Molecules and Atomic Nuclei," James Franck Institute, University of Chicago, Chicago, Illinois, U.S.A., March 15, 2005.

67.** "New Alternatives for Accurate Quantum Calculations for Molecular Systems: Bond Breaking, Diradicals, and Excited Electronic States," Department of Chemistry, Oakland University, Rochester, Michigan, U.S.A., April 6, 2005.

68.** "New Alternatives for Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Bond Breaking and Diradicals to Excited States in Molecules and Atomic Nuclei," Department of Chemistry and Theoretical Chemistry Institute, University of Wisconsin–Madison, Madison, U.S.A., May 9, 2005.

69.** "Renormalized and Active-Space Coupled-Cluster Methods: Two Approaches to Electronic Quasi-Degeneracies and Open-Shell Problems," Fifth Congress of the International Society for Theoretical Chemical Physics (ICTCP-V), New Orleans, Louisiana, U.S.A., July 20-26, 2005 [invited plenary lecture].

70.** "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States," The symposium "Theoretical Determination of Energy Landscapes: Methodology and Applications," 230th American Chemical Society National Meeting, Washington, DC, U.S.A., August 28 - September 1, 2005.

71.** "Renormalized and Active-Space Coupled-Cluster Methods: Two Approaches to Quasi-Degeneracies and Open-Shell Problems," Conference on Microscopic Approaches to Many-Body Theory, in honor of Professor Raymond Bishop, The University of Manchester, Manchester, U.K., August 31 - September 3, 2005.

72.** "Active-Space Coupled-Cluster Method: An Inexpensive and Highly Accurate Approach to Electronic Quasi-Degeneracies and Open-Shell Problems," Tenth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-X, Carthage, Tunisia, September 1-7, 2005.

73.** "New Alternatives for Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Bond Breaking and Biradicals to Excited States in Molecules and Atomic Nuclei," Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University, Kyoto, Japan, October 6, 2005.

74.** "Advances in Electronic Structure Theory: Multi-Reference Coupled-Cluster Methods," Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan, October 31, 2005.

75.** "New Alternatives for Accurate Quantum Calculations for Molecular Systems: From Bond Breaking and Biradicals to Excited Electronic States," Department of Applied Chemistry, School of Engineering, The University of Tokyo, Tokyo, Japan, November 18, 2005.

76.** "New Alternatives for Accurate Quantum Calculations for Molecular Systems: From Bond Breaking and Biradicals to Excited Electronic States," 9th Quantum Chemistry Seminar, Department of Chemistry, School of Science and Engineering, Waseda University, Tokyo, November 19, 2005.

77.** "New Alternatives for Accurate Quantum Calculations for Molecular Systems: From Bond Breaking and Biradicals to Excited Electronic States," Department of Knowledge-Based Information Engineering, Toyohashi University of Technology, Toyohashi, Japan, November 24, 2005.

78.** "New Alternatives for Accurate Quantum Calculations for Molecular Systems: From Bond Breaking and Biradicals to Excited Electronic States," Department of Chemistry, University of Coimbra, Portugal, March 23, 2006.

79.** "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [invited plenary lecture].

80.** "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," Unidad Asociada Universidad Autónoma de Madrid – Consejo Superior de

Investigaciones Cientificas (UAM-CSIC), Instituto de Matemáticas y Física Fundamental, Departamento de Física Atómica, Molecular y de Agregados (Department of Atomic, Molecular, and Cluster Physics), Madrid, Spain, July 14, 2006.

81.** "Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Bond Breaking and Electronic Excitations in Molecules to Properties of Atomic Nuclei," The Centro Internacional de Matemática Workshop "Mathematics in Chemistry," Lisbon, Portugal, July 19-21, 2006.

82.** "Advances in Electronic Structure Theory: Single-Reference Coupled-Cluster Methods for Multi-Reference Problems," Sixth Canadian Computational Chemistry Conference (CCCC6), Vancouver, British Columbia, Canada, July 26-30, 2006 [invited plenary lecture].

83.** "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," Eleventh European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XI, St. Petersburg, Russia, August 20-25, 2006.

84.** "Accurate Quantum Calculations for Many-Body Systems: From Reaction Mechanisms in Organic and Bioinorganic Chemistries to Properties of Atomic Nuclei," Michigan State University High Performance Computing Center 2006 Symposium, East Lansing, Michigan, U.S.A., October 7, 2006.

85.** "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," Department of Chemistry, The University of Western Ontario, London, Ontario, Canada, November 8, 2006.

86.** "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada, November 10, 2006.

87.** "Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Reaction Pathways in Chemistry to Properties of Atomic Nuclei," the S.R. Palit Memorial Lecture, Indian Association for the Cultivation of of Science, Kolkata (Calcutta), India, January 9th, 2007.

88.** "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," International Conference "Recent Trends in Many-Body Methods for Electronic Structure and Properties of Atoms and Molecules," Bhubaneswar and Puri, Orissa, India, January 11-13, 2007.

89.** "Active-Space Coupled-Cluster Methods for Bond Breaking, Excited Electronic States, and Open-Shell Systems," International Conference "Practicing Chemistry with Theoretical Tools, on the Occasion of Professor Mark S. Gordon's 65th Birthday," Kihei, Hawaii, U.S.A., January 15-18, 2007.

90.** "Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Reaction Pathways in Chemistry to Properties of Atomic Nuclei," Department of Chemistry, Western Michigan University, Kalamazoo, Michigan, U.S.A., April 2, 2007.

91.** "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," 39th Midwest Theoretical Chemistry Conference, Indiana University, Bloomington, Indiana, U.S.A., June 28-30, 2007.

92.** "Coupled-Cluster Theory: An Overview of the Basic Formalism and Applications to Molecular and Nuclear Structure Problems," Workshop on Advanced Many-body Methods for Nuclear Structure European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Trento, Italy, July 2-6, 2007.

93.** "Coupled-Cluster Theory: Basic Formalism, Recent Developments, and Applications to Molecular and Nuclear Structure Problems," Institut für Kernphysik, Fachbereich Physik, Technische Universität Darmstadt, Darmstadt, Germany, August 29, 2007.

94.** "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Applications to Radicals, Biradicals, and Bond Breaking," Twelfth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XII, London, U.K., August 30 - September 5, 2007.

95.** "Coupled-Cluster Theory: Basic Formalism, Recent Developments, and Applications to Molecular and Nuclear Structure Problems," Faculty of Chemistry, University of Wrocław, Wrocław, Poland, September 10, 2007.

96.** "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Applications to Radicals, Biradicals, Reaction Pathways, and Photochemistry," "IXth International Conference on Molecular Spectroscopy: From Molecules to Molecular Biological Systems and Molecular Materials, Role of Molecular Interactions and Recognition," Wrocław – Lądek-Zdrój, Poland, September 13-18, 2007.

97.** "Coupled-Cluster Theory: Basic Formalism, Recent Developments, and Applications to Molecular and Nuclear Structure Problems," Department of Chemistry, Wake Forest University, Winston-Salem, North Carolina, November 28, 2007.

98.** "Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Reaction Pathways in Chemistry to Properties of Atomic Nuclei," the Computational Materials Seminar Series, Department of Chemistry and Chemical Biology, Cornell University, Ithaca, New York, February 7, 2008.

99.** "Coupled-Cluster Calculations for Many-Electron and Other Many-Fermion Systems: From Reaction Pathways in Chemistry to Atomic Nuclei," Department of Chemistry, University of Michigan, Ann Arbor, Michigan, March 20, 2008.

100.** "Coupled-Cluster Calculations for Many-Electron and Other Many-Fermion Systems: From Reaction Pathways in Chemistry to Atomic Nuclei," Chemistry and Physics Colloquium, Michigan Technological University, Houghton, Michigan, March 27, 2008.

101.** "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell Systems," The symposium "Electronic Structure and Reaction Dynamics of Open-shell Species," 235th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., April 6-10, 2008.

102.** "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Molecular Applications," Center for Computational Chemistry, University of Georgia, Athens, Georgia, U.S.A., May 6, 2008.

103.** "Some Developments in Multi-Reference Coupled-Cluster Theory and Applications of Coupled-Cluster Methods to Atomic Nuclei," Center for Computational Chemistry, University of Georgia, Athens, Georgia, U.S.A., May 7, 2008.

104.** "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," Sixth Congress of the International Society for Theoretical Chemical Physics (ICTCP-VI), Vancouver, British Columbia, Canada, July 19-24, 2008 [invited plenary lecture].

105.** "Coupled-Cluster Theory: A Brief Overview of Modern Methods and Applications to Nuclear Structure," the WE-Heraeus-Seminar "Ab-Initio Nuclear Structure - Where do we stand?", Bad Honnef, Germany, July 28-30, 2008.

106.** "Coupled-Cluster Theory: An Overview of Modern Methods and Applications to Nuclear and Electronic Structure," Institut für Kernphysik, Fachbereich Physik, Technische Universität Darmstadt, Darmstadt, Germany, August 4, 2008.

107.** "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2008), Sydney, Australia, September 14-19, 2008.

108.** "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," The International Conference "Theory and Applications of Computational Chemistry 2008 (TACC 2008)," Shanghai, China, September 23-27, 2008 [invited plenary lecture].

109.** "Extending Electronic Structure Theory to Complex Molecular Problems: Local Correlation Coupled-Cluster and Correlation Energy Scaling Methodologies," The symposium "Advances in Electronic Structure Theory and First Principles Dynamics," 237th American Chemical Society National Meeting, Salt Lake City, Utah, U.S.A., March 22-26, 2009.

110.** "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States," 30th Annual Combustion Research Meeting, Airlie Conference Center, Warrenton, Virginia, May 26-29, 2009.

111.** "Coupled-Cluster Theory: From Quantum Chemistry to Applications in Nuclear Physics," International Workshop "Linking Nuclei, Molecules, and Condensed Matter: Computational Quantum Many-Body Approaches," European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Trento, Italy, July 6-10, 2009.

112.** "Dealing with Strong Electron Correlations in Quantum Chemistry via Renormalized, Active-Space, and Multi-Reference Coupled-Cluster Methods," The symposium "New Developments in Strongly Correlated Electrons," 238th American Chemical Society National Meeting, Washington, DC, U.S.A., August 16-20, 2009.

113.** "Extending Electronic Structure Theory to Complex Molecular Problems: Local Correlation Coupled-Cluster and Correlation Energy Scaling Methodologies," Fourteenth International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XIV, San Lorenzo de El Escorial, Madrid, Spain, September 13-19, 2009.

114.** "Extending *Ab Initio* Electronic Structure Theory to Complex Molecular Problems: Local Coupled-Cluster and Correlation Energy Scaling Methodologies," Department of Chemistry, Iowa State University, Ames, Iowa, U.S.A., October 2, 2009.

115.** "Dealing with Strong Electron Correlations in Quantum Chemistry via Renormalized, Active Space, and Multireference Coupled-Cluster Methods," An International Symposium "Recent Advances in Many Electron Theories," Shankarpur, West Bengal, India, January 5-7, 2010.

116.** "Extending Ab Initio Electronic Structure Theory to Complex Molecular Problems: Local Coupled-Cluster and Correlation Energy Scaling Methodologies," Physical Chemistry Division, National Chemical Laboratory, Pune, India, January 9, 2010.

117.** "Extending Ab Initio Electronic Structure Theory to Complex Molecular Problems: Local Coupled-Cluster and Correlation Energy Scaling Methodologies," Institute Colloquium, Indian Association for the Cultivation of of Science, Kolkata (Calcutta), India, January 11th, 2010.

118.** "Extending Ab Initio Electronic Structure Theory to Complex Molecular Problems: Local Coupled-Cluster Methodology and Its Multi-Level Generalizations," Center for Nanomaterials Design and Assembly Seminar, Michigan State University, East Lansing, Michigan, U.S.A., January 21, 2010.

119.** "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," the 50th Sanibel Symposium, St. Simons Island, Georgia, U.S.A., February 24-March 2, 2010.

120.** "Extending Ab Initio Electronic Structure Theory to Complex Molecular Problems: Local Coupled-Cluster and Correlation Energy Scaling Methodologies," The William R. Wiley Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington, U.S.A., May 12, 2010 [Distinguished Seminar].

121.** "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," International conference "Molecular Quantum Mechanics: From Methylene to DNA and Beyond" honoring Professor Henry F. Schaefer's work, University of California at Berkeley, Berkeley, California, May 24-29, 2010.

122.** "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," 17th Canadian Symposium on Theoretical Chemistry, Edmonton, Alberta, Canada, July 25-30, 2010.

123.** "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," Fifteenth International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XV, Magdalene College, Cambridge University, Cambridge, U.K., August 31 - September 5, 2010.

124.** "Dealing with Chemical Reaction Pathways and Electronic Excitations in Molecular Systems via Renormalized and Active-Space Coupled-Cluster Methods," 18th European Conference on Dynamics of Molecular Systems, MOLEC XVIII, Curia, Portugal, September 5-10, 2010.

125.** "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," 9th Central European Symposium on Theoretical Chemistry, CESTC 2010, Nový Smokovec, Slovakia, September 12-15, 2010.

126.** "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Molecular Applications," Center for Advanced Computational Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia, September 17, 2010.

127.** "Extending Ab Initio Electronic Structure Theory to Large Molecular Systems: Local Correlation Coupled-Cluster Methods and their Multi-level Generalizations," Institute for Cyber Enabled Research (iCER), Michigan State University, East Lansing, Michigan, U.S.A., September 23, 2010.

128.** "Dealing with Chemical Reaction Pathways and Electronic Excitations in Molecular Systems via Renormalized and Active-Space Coupled-Cluster Methods," 8th International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2010), symposium "Methods in Quantum Chemistry" in honor of Jiri Čížek and Josef Paldus, Kos, Greece, October 3-8, 2010 [invited featured lecture].

129.** "Extending Ab Initio Electronic Structure Theory to Complex Molecular Problems: Local Coupled-Cluster and Correlation Energy Scaling Methodologies," Institute of Physical and Theoretical Chemistry, Faculty of Chemistry, Wrocław University of Technology, Wrocław, Poland, October 11, 2010.

130.** "Dealing with Chemical Reaction Pathways and Electronic Excitations in Molecular Systems via Renormalized and Active-Space Coupled-Cluster Methods," Faculty of Chemistry, University of Wrocław, Wrocław, Poland, October 11, 2010.

131.** "Extending Ab Initio Electronic Structure Theory to Complex Molecular Problems: Local Coupled-Cluster and Correlation Energy Scaling Methodologies," Faculty of Chemistry, University of Warsaw, Warsaw, Poland, October 13, 2010.

132.** "Coupled-Cluster Theory: From Quantum Chemistry to Applications in Nuclear Physics," Faculty of Physics, University of Warsaw, Warsaw, Poland, October 14, 2010.

133.** "Dealing with Chemical Reaction Pathways and Electronic Excitations in Molecular Systems via Renormalized and Active-Space Coupled-Cluster Methods," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Warsaw, Poland, October 14, 2010.

134.** "Extending Ab Initio Electronic Structure Theory to Large Molecular Systems: Local Correlation Coupled-Cluster Methods and their Multi-level Generalizations," Department of Chemistry, Emory University, Atlanta, Georgia, U.S.A., December 6, 2010.

135.** "Dealing with Chemical Reaction Pathways and Electronic Excitations in Molecular Systems via Renormalized and Active-Space Coupled-Cluster Methods," Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., February 25, 2011.

136.** "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," The symposium "Fragment and Local Orbital Methods in Electronic Structure Theory," 241st American Chemical Society National Meeting, Anaheim, California, U.S.A., March 27-31, 2011.

137.** "Dealing with Chemical Reaction Pathways and Electronic Excitations in Molecular Systems via Renormalized and Active-Space Coupled-Cluster Methods," Department of Chemistry and Center for Advanced Scientific Computing and Modeling, University of North Texas, Denton, Texas, U.S.A., May 11, 2011.

138.** "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," 11th Annual CERMM Symposium, Centre for Research in Molecular Modeling, Concordia University, Montreal, Canada, June 4-5, 2011 [invited keynote lecture].

139.** "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," 94th Canadian Chemistry Conference and Exhibition, General Physical, Theoretical, and Computational Chemistry Session, Montreal, Canada, June 5-9, 2011.

140.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems and their Multi-Level Generalizations," Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2011), Santiago de Compostela, Spain, July 17-22, 2011.

141.** "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," WATOC 2011 Satellite Conference "Strongly Correlated Systems, Cooperativity, and Valence-Bond Theory," A Coruña, Spain, July 23-25, 2011.

142.** "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," The symposium "Reduced Density Matrices in Quantum Chemistry," 242nd American Chemical Society National Meeting, Denver, Colorado, U.S.A., August 28 - September 1, 2011.

143.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems and their Multi-Level Generalizations," The symposium "Quantum Chemistry: Methodology," 242nd American Chemical Society National Meeting, Denver, Colorado, U.S.A., August 28 - September 1, 2011.

144.** "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," The symposium "Quantum Chemistry: DFT," 242nd American Chemical Society National Meeting, Denver, Colorado, U.S.A., August 28 - September 1, 2011.

145.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems and their Multi-Level Generalizations," Seventh Congress of the International Society for Theoretical Chemical Physics (ICTCP-VII), Tokyo, Japan, September 2-8, 2011.

146.** "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," XVI-th International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XVI, Kanazawa, Japan, September 11-17, 2011.

147.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems and their Multi-Level Generalizations," Department of Chemistry, Oakland University, Rochester, Michigan, U.S.A., November 9, 2011.

148.** "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," An International Symposium "Recent Advances in Many Electron Theories II, 2011," Puri, Orissa, India, December 1-4, 2011.

149.** "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," The Fifth Asian Pacific Conference of Theoretical and Computational Chemistry (APCTCC 2011), Rotorua, New Zealand, December 9-13, 2011.

150.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems and their Multi-Level Generalizations," Centre for Theoretical Chemistry and Physics (CTCP), The New Zealand Institute for Advanced Study (NZIAS), Massey University, Auckland, New Zealand, December 14, 2011.

151.** "Coupled-Cluster Theory: From Quantum Chemistry to Applications in Nuclear Physics," Department of Physics and Astronomy, University of Louisville, Lousville, Kentucky, March 7, 2012.

152.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems and their Multi-Level Generalizations," Department of Chemistry, University of Louisville, Lousville, Kentucky, March 9, 2012.

153.** "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States (Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods)," 33rd Annual Combustion Research Meeting, Bolger Center, Potomac, Maryland, U.S.A., May 29 - June 1, 2012.

154.** "Recent Progress in Renormalized and Active-Space Coupled-Cluster Methods," The symposium "Coupled-Cluster Theory and Related Methods," A Satellite Symposium to the 14th International Congress of Quantum Chemistry, Boulder, Colorado, U.S.A., July 1-3, 2012.

155.** "Renormalized and Active-Space Coupled-Cluster Methods: Key Concepts and Recent Advances," 23rd Quantum Chemistry Seminar, Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University, Tokyo, July 31, 2012.

156.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems and their Multi-Level Generalizations," 23rd Quantum Chemistry Seminar, Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University, Tokyo, August 1, 2012.

157.** "Renormalized and Active-Space Coupled-Cluster Methods: Key Concepts and Recent Advances," Quantum Chemistry Research Institute, Kyoto, Japan, August 7, 2012.

158.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems and their Multi-Level Generalizations," Quantum Chemistry Research Institute, Kyoto, August 7, 2012.

159.** "Renormalized and Active-Space Coupled-Cluster Methods: Key Concepts and Recent Advances," Institute for Molecular Science, National Institutes of Natural Sciences, Okazaki, Japan, August 10, 2012.

160.** "Multi-level Extensions of the Cluster-in-Molecule Local Correlation Methodology Aimed at Chemical Reaction Pathways Involving Large Molecular Systems," The symposium "Bridging the Gap between Ab Initio and Classical Simulations," 244th American Chemical Society National Meeting, Philadelphia, Pennsylvania, U.S.A., August 19-23, 2012.

161.** "Combining Active-Space Coupled-Cluster Methods with Moment Energy Corrections via the CC($P;Q$) Methodology, with Benchmark Calculations for Bond Breaking and Biradical Transition States," The symposium "Exploring Potential Energy Surfaces in Quantum Chemistry: A Tribute to H. Bernhard Schlegel," 244th American Chemical Society National Meeting, Philadelphia, Pennsylvania, U.S.A., August 19-23, 2012.

162.** "Renormalized and Active-Space Coupled-Cluster Methods: Key Concepts and Recent Advances," Department of Chemistry, Wayne State University, Detroit, Michigan, U.S.A., September 12, 2012.

163.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems," 844th IMS Colloquium, Institute for Molecular Science, National Institutes of Natural Sciences, Okazaki, Japan, February 15, 2013.

164.** "Renormalized and Active-Space Coupled-Cluster Methods: Key Concepts and Recent Advances," Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan, February 27, 2013.

165.** "Renormalized and Active-Space Coupled-Cluster Methods: Key Concepts and Recent Advances," Catalysis Research Center, Hokkaido University, Sapporo, Japan, March 19, 2013.

166.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems," Catalysis Research Center, Hokkaido University, Sapporo, Japan, March 19, 2013.

167.** "Renormalized and Active-Space Coupled-Cluster Methods: Key Concepts and Recent Advances," Graduate School of System Informatics, Kobe university Kobe, Japan, March 25, 2013.

168.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems," 5th Computational Molecular Science Seminar, RIKEN Advanced Institute for Computational Science, Kobe, Japan, March 26, 2013.

169.** "Accurate Characterization of Reaction Pathways Relevant to Combustion and Electronic Excitations in Radicals and Biradicals via Renormalized and Active-Space Coupled-Cluster Theories, their Merger, and Open-Shell Extensions," The symposium on Combustion Chemistry, 245th American Chemical Society National Meeting, New Orleans, Lousiana, U.S.A., April 7-11, 2013.

170.** "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," The symposium "Quantum Chemistry: Methodology," 245th American Chemical Society National Meeting, New Orleans, Lousiana, U.S.A., April 7-11, 2013.

171.** "The Cobalt-Methyl Dissociation and Electronic Transitions in Methylcobalamin: Insights from the Coupled-cluster, Multireference Perturbation Theory, and Density Functional Theory Calculations," The symposium "Bioinorganic Chemistry: Proteins and Enzymes and Model Systems," 245th American Chemical Society National Meeting, New Orleans, Lousiana, U.S.A., April 7-11, 2013.

172.** "Recent Progress in the Active-Space Electron-Attached and Ionized Equation-of-Motion Coupled-Cluster Methodologies," 7th International Conference "Molecular Quantum Mechanics" entitled "Electron Correlation: The Many-Body Problem at the Heart of Chemistry," in honor of Professor Rodney J. Bartlett, Lugano, Switzerland, June 2-7, 2013.

173.** "Renormalized and Active-Space Coupled-Cluster Methods: Key Concepts and Recent Advances," Department of Physical Chemistry, University of Geneva, Switzerland, June 11, 2013.

174.** "The Cobalt-Methyl Dissociation and Electronic Transitions in Methylcobalamin: Insights from Coupled-Cluster, Multireference Perturbation Theory, and Density Functional Theory Calculations," Department of Physical Chemistry, University of Geneva, Switzerland, June 11, 2013.

175.** "Renormalized and Active-Space Coupled-Cluster Methods: Key Concepts and Recent Advances," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Warsaw, Poland, August 23, 2013.

176.** "Recent Progress in the Active-Space Electron-Attached and Ionized Equation-of-Motion Coupled-Cluster Methodologies," Eighth Congress of the International Society for Theoretical Chemical Physics (ISTCP-VIII), Budapest, Hungary, August 25-31, 2013.

177.** "Single-Reference Coupled-Cluster Methods for Multi-Reference Molecular Problems," 6th Conference "Current Trends in Theoretical Chemistry" (CTTC VI), Cracow, Poland, September 1-5, 2013.

178.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems," Faculty of Chemistry, Jagiellonian University, Cracow, Poland, September 6, 2013.

179.** "Renormalized and Active-Space Coupled-Cluster Methods: Key Concepts and Recent Advances," Institute of Chemistry, University of Silesia, Katowice, Poland, September 6, 2013.

180.** "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems," Institute of Physical and Theoretical Chemistry, Faculty of Chemistry, Wrocław University of Technology, Wrocław, Poland, September 9, 2013.

181.** "The Cobalt-Methyl Dissociation and Electronic Transitions in Methylcobalamin: Insights from Coupled-cluster, Multireference Perturbation Theory, and Density Functional Theory Calculations," Institute of Physical and Theoretical Chemistry, Faculty of Chemistry, Wrocław University of Technology, Wrocław, Poland, September 10, 2013.

182.** "Understanding Photochemistry and Photo-ionization Dynamics with Highly Correlated Electronic Structure Methods: Two Examples that Highlight the Transformative Role of Theory in the Interpretation of Experimental Observations," XVIII-th International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XVIII), Paraty (Rio de Janeiro), Brazil, December 1-7, 2013.

183.** "Understanding Photochemistry and Photo-ionization Dynamics with Highly Correlated Electronic Structure Methods: Two Examples that Highlight the Transformative Role of Theory in the Interpretation of Experimental Observations," The symposium "A Little Insight Goes a Long Way," 247th American Chemical Society National Meeting, Dallas, Texas, U.S.A., March 16-20, 2014.

184.** "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(P;Q) Methodology: Connected Triple and Quadruple Excitations," The symposium "Quantum Chemistry: Methodology," 247th American Chemical Society National Meeting, Dallas, Texas, U.S.A., March 16-20, 2014.

185.** "Utility of New Generations of Coupled-Cluster Methods and Algorithms in Catalytic and Structural Properties of Gold Nanoparticles," The symposium "Quantum Chemistry: Applications," 247th American Chemical Society National Meeting, Dallas, Texas, U.S.A., March 16-20, 2014.

186.** "The Cobalt-Methyl Dissociation and Electronic Transitions in Methylcobalamin: Insights from Coupled-Cluster, Multireference Perturbation Theory, and Density Functional Theory Calculations," Department of Chemistry, Washington University in St. Louis, St. Louis, Missouri, U.S.A., May 22, 2014.

187.** "Renormalized and Active-Space Coupled-Cluster Methods: Key Concepts, Recent Advances, and Examples of Molecular Applications," Department of Chemistry, Washington University in St. Louis, St. Louis, Missouri, U.S.A., May 23, 2014.

188.** "Single-Reference Coupled-Cluster Methods for Multi-Reference Molecular Problems," Nordita program on "Computational Challenges in Nuclear and Many-Body Physics," Stockholm, Sweden, September 15 - October 10, 2014.

189.** "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(P;Q) Methodology," Tenth Triennial Congress of the World Association

of Theoretical and Computational Chemists (WATOC 2014), Santiago, Chile, October 5-10, 2014.

190.** "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(P;Q) Methodology," The Fourteenth Theoretical Chemistry Symposium (TCS 2014), Pune, India, December 18-21, 2014 [invited keynote lecture].

191.** "Understanding Photochemistry and Photoelectron Spectra with Highly Correlated Electronic Structure Methods Based on Coupled-Cluster Theory," The symposium "Modeling Excited States of Complex Systems," 249th American Chemical Society National Meeting, Denver, Colorado, U.S.A., March 22-26, 2015.

192.** "Aerobic Oxidation of Methanol to Formic Acid on Au_8^-: Benchmark Analysis Based on Completely Renormalized Coupled-Cluster and Density Functional Theory Calculations," The symposium "Computational Chemical Dynamics: Advancing Our Understanding of Chemical Processes in Gas-Phase, Biomolecular and Condensed-Phase Systems," 249th American Chemical Society National Meeting, Denver, Colorado, U.S.A., March 22-26, 2015.

193.** "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(P;Q) Methodology: Ground and Excited States," The symposium "Quantum Chemistry: Methodology," 249th American Chemical Society National Meeting, Denver, Colorado, U.S.A., March 22-26, 2015.

194.** "Molecular Systems from the Equation-of-Motion Coupled-Cluster Theory" or "Understanding Electronic Excitation, Multi-Photon Ionization, and Photo-Electron Spectra with the Equation-of-Motion Coupled-Cluster Theory," Workshop of the Espace de Structure Nucléaire Théorique on "Near-Degenerate Systems in Nuclear Structure and Quantum Chemistry from Ab-Initio Many-Body Methods," CEA Saclay, France, March 30 - April 2, 2015.

195.** "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems," The symposium "Recent Advances in Electronic Structure Theory (RAEST2015)," A Satellite Symposium to the 15th International Congress of Quantum Chemistry, Nanjing, China, June 1-6, 2015.

196.** "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Theories for High-Accuracy *Ab Initio* Computations of Chemical Reaction Profiles Involving Biradical Transition States and Electronic Spectra of Radical and Polyradical Species," The symposium "From Diradicals and Polyradicals to Functionalized Materials: Theory Meets Experiment," 250th American Chemical Society National Meeting, Boston, Massachusetts, U.S.A., August 16-20, 2015.

197.** "Understanding Photochemistry, Multi-photon Ionization, and Photoelectron Spectra with the Equation-of-Motion Coupled-Cluster Theory," Center of Research Excellence in Complex Materials, Michigan State University, East Lansing, Michigan, U.S.A., September 10, 2015.

198.** "Understanding Photochemistry, Multi-photon Ionization, and Photoelectron Spectra with the Equation-of-Motion Coupled-Cluster Theory," Department of Chemistry and

Theoretical Chemistry Institute, University of Wisconsin–Madison, Madison, U.S.A., September 24, 2015.

199.** "Utility of New Generations of Coupled-Cluster Methods and Algorithms in Catalytic, Structural, and Optical Properties of Gold Nanoparticles," The symposium "Interplay between Theory and Experiment in Catalytic Research," the 2015 International Chemical Congress of Pacific Basin Societies (Pacifichem 2015), Honolulu, Hawaii, U.S.A., December 15-20, 2015.

200.** "Understanding Photochemistry, Multi-photon Ionization, and Photoelectron Spectra with the Equation-of-Motion Coupled-Cluster Theory," Department of Physics, Washington University in St. Louis, St. Louis, Missouri, U.S.A., January 28, 2016.

201.** "Utility of New Generations of Coupled-Cluster Methods and Algorithms in the Examination of Catalytic, Structural, and Optical Properties of Gold Nanoparticles," Department of Chemistry, Washington University in St. Louis, St. Louis, Missouri, U.S.A., February 11, 2016.

202.** "Coupled-Cluster Interpretation of the Photoelectron Spectra of Ag_3^- and Au_3^-," 26th Austin Symposium on Molecular Structure and Dynamics, Dallas, Texas, U.S.A., March 5-7, 2016.

203.** "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States (Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: CC(P;Q) Formalism)," 2nd Computational and Theoretical Chemistry Research PI Meeting, Gaithersburg, Maryland, U.S.A., May 15-18, 2016.

204.** "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems," TSRC Workshop "Low-Scaling and Unconventional Electronic Structure Techniques" (LUEST 2016), 3rd edition, Telluride, Colorado, U.S.A., June 1-5, 2016.

205.** "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: CC(P;Q) Formalism," Ninth Congress of the International Society for Theoretical Chemical Physics (ISTCP-IX), Grand Forks, North Dakota, U.S.A., July 17-22, 2016.

206.** "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: CC(P;Q) Formalism," The International Conference "Theory and Applications of Computational Chemistry 2016 (TACC 2016)," Seattle, Washington, August 28 - September 2, 2016.

207.** "Understanding Photochemistry and Photoelectron Spectra with Highly Correlated Electronic Structure Methods based on Coupled-Cluster Theory," 7th Conference "Current Trends in Theoretical Chemistry" (CTTC VII), Cracow, Poland, September 4-8, 2016.

208.** "Utility of New Generations of Coupled-Cluster Methods and Algorithms in the Examination of Catalytic, Structural, and Optical Properties of Gold and Silver Nanoparticles," Institute of Chemistry, University of Silesia, Katowice, Poland, September 9, 2016.

209.** "The Cobalt-Methyl Dissociation and Electronic Transitions in Methylcobalamin: Insights from Coupled-Cluster, Multireference Perturbation Theory, and Density Functional Theory Calculations," Department of Chemistry and Institute of Physics, Lódź University of Technology, Lódź, Poland, September 12, 2016.

210.** "Coupled-Cluster Theory: From Quantum Chemistry to Applications in Nuclear Physics," Department of Chemistry and Institute of Physics, Lódź University of Technology, Lódź, Poland, September 12, 2016.

211.** "Utility of New Generations of Coupled-Cluster Methods and Algorithms in the Examination of Catalytic, Structural, and Optical Properties of Gold and Silver Nanoparticles," Institute of Physical and Theoretical Chemistry, Faculty of Chemistry, Wrocław University of Technology, Wrocław, Poland, September 15, 2016.

212.** "Quantum Chemistry and Physics," The Adam Mickiewicz High School No. 3, Wrocław, Poland, September 16, 2016 (special guest lecture on the occasion of the 70th anniversary of establishing the school).

213.** "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: CC(P;Q) Formalism," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Warsaw, Poland, September 19, 2016.

214.** "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," EMN Meeting on Computation and Theory (Energy, Materials, and Nanotechnology), workshop "Novel Electron Correlation Methods for Complex Systems," Las Vegas, Nevada, U.S.A., October 10-14, 2016.

215.** "Single-Reference Methods for Multi-Reference Problems: Renormalized and Active-Space Coupled-Cluster Approaches and CC(P;Q) Formalism," Department of Chemistry (Professor Gustavo Scuseria's Group), Rice University, Houston, Texas, U.S.A., October 25, 2016.

216.** "Understanding Photochemistry and Photoelectron Spectra with Highly Correlated *Ab Initio* Methods of Electronic Structure Theory," Department of Chemistry, Rice University, Houston, Texas, U.S.A., October 26, 2016.

217.** "Coupled-Cluster Interpretation of the Photoelectron Spectra of Ag_3^- and Au_3^-," GAMESS*7557*SSEMAG Palindromic Birthday Theory Symposium, on the Occasion of Professor Mark S. Gordon's 75th and Professor Kim K. Baldridge 57th Birthdays," Lihue, Hawaii, U.S.A., January 16-18, 2017.

218.** "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," An International Conference "Recent Advances in Many-Electron Theory (RAMET-2017)," Goa, India, February 9-12, 2017.

219.** "The 1966 *Journal of Chemical Physics* Article by Jiří Čížek: What Is in It and Why Is It so Important," the 57th Sanibel Symposium, a special symposium recognizing the 50th Anniversary of Jiří Čížek's 1966 Paper on Coupled-Cluster Theory, St. Simons Island, Georgia, U.S.A., February 19-24, 2017.

220.** "Understanding Photochemistry and Photoelectron Spectra with Coupled-Cluster Theory," The Lawrence J. Schaad Lectureship in Theoretical Chemistry (the fourth lecture in a series), Department of Chemistry, Vanderbilt University, Nashville, Tennessee, U.S.A., April 5, 2017.

221.** "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: CC(P;Q) Formalism," The symposium "Electronic Structure of Complex Chemical Systems," 254th American Chemical Society National Meeting, Washington, DC, U.S.A., August 20-24, 2017.

222.** "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," PHYS Awards Symposium, 254th American Chemical Society National Meeting, Washington, DC, U.S.A., August 20-24, 2017.

223.** "Stochastic CC(P;Q) Theory: Converging High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," Eleventh Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2017), Munich, Germany, August 27 - September 1, 2017.

224.** "High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," 15th Central European Symposium on Theoretical Chemistry, CESTC 2017, Wisła, Poland, September 3-6, 2017.

225.** "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," Department of Chemistry, University of Nevada, Reno, Nevada, U.S.A., October 20, 2017.

226.** "High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," 27th Austin Symposium on Molecular Structure and Dynamics, Dallas, Texas, U.S.A., March 3-5, 2018.

227.** "New Paradigm in Quantum Chemistry: Accurate Electronic Energetics by Stochastic Wave Function Sampling Followed by Deterministic Coupled-Cluster Computations," Department of Chemistry, Washington University in St. Louis, St. Louis, Missouri, U.S.A., March 6, 2018.

228.** "Introduction to Single-Reference Many-Body Perturbation Theory and its Diagrammatic Representation," Workshop of the Espace de Structure Nucléaire Théorique on "Many-Body Perturbation Theories in Modern Quantum Chemistry and Nuclear Physics," CEA Saclay, France, March 26-30, 2018.

229.** "Perturbative Corrections to Non-perturbative Methods" or "High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," Workshop of the Espace de Structure Nucléaire Théorique on "Many-Body Perturbation Theories in Modern Quantum Chemistry and Nuclear Physics," CEA Saclay, France, March 26-30, 2018.

230.** "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," NSCL Theory Seminar, National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Michigan, U.S.A., April 10, 2018.

231.** "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," Chemical Theory Center, University of Minnesota, Minneapolis, Minnesota, U.S.A., April 20, 2018.

232.** "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," 4th Computational and Theoretical Chemistry Research PI Meeting, Gaithersburg, Maryland, U.S.A., May 21-24, 2018.

233.** "High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," TSRC Workshop "Low-Scaling and Unconventional Electronic Structure Techniques" (LUEST 2018), 4th edition, Telluride, Colorado, U.S.A., June 4-8, 2018.

234.** "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," The joint Annual Workshop on Recent Developments in Electronic Structure Methods (ES18) and Penn Conference in Theoretical Chemistry (PCTC18), Philadelphia, Pennsylvania, U.S.A., June 10-14, 2018.

235.** "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," The symposium "Strong Correlation in Electronic Structure Theory," A Satellite Symposium to the 16th International Congress of Quantum Chemistry, Strasbourg, France, June 24-27, 2018.

236.** "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," 28th Canadian Symposium on Theoretical and Computational Chemistry (CSTCC 2018), Windsor, Ontario, Canada, July 15-19, 2018.

237.** "Toward Exact Quantum Chemistry: Accurate Electronic Energies by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Department of Chemistry, North Carolina State University, Raleigh, North Carolina, U.S.A., October 11, 2018.

238.** "Toward Exact Quantum Chemistry: Accurate Electronic Energies by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," The international conference "Quantum International Frontiers 2018," Changsha, Hunan Province, China, October 17-21, 2018 [invited Frontier Lecture].

239.** "Toward Exact Quantum Chemistry: Accurate Electronic Energies by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Center for Computational Chemistry, University of Georgia, Athens, Georgia, U.S.A., October 30, 2018.

240.** "Toward Exact Quantum Chemistry: Accurate Electronic Energies by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Department of Chemistry, Emory University, Atlanta, Georgia, U.S.A., October 31, 2018.

241.** "Toward Exact Quantum Chemistry: Accurate Electronic Energies by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Department of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia, U.S.A., November 1, 2018.

242.** "Toward Exact Quantum Chemistry: Accurate Electronic Energies by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Department of Chemistry, Virginia Polytechnic Institute and State University, Blacksburg, Virginia, U.S.A., November 12, 2018.

243.** "Toward Exact Quantum Chemistry by Combining Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Mainz-Kobe Joint Workshop on "Solving the Full Configuration Interaction Problem," RIKEN Center for Computational Science, Kobe, Japan, November 26-27, 2018 [teleconference session].

244.** "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Department of Chemistry, University of Michigan, Ann Arbor, Michigan, U.S.A., February 28, 2019.

245.** "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," TSRC Workshop "New Frontiers in Electron Correlation," 2nd edition, Telluride, Colorado, U.S.A., June 10-14, 2019.

246.** "Quantum Chemistry and Physics: My Academic Trajectory and Most Recent Interests," The 56th Meeting of the International Academy of Quantum Molecular Science (IAQMS), Menton, France, July 6-7, 2019.

247.** "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Tenth Congress of the International Society for Theoretical Chemical Physics (ISTCP-X), symposium entitled "Emergent Electronic Structure Methods," Tromsø, Norway, July 11-17, 2019.

248.** "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," 8th Conference "Current Trends in Theoretical Chemistry" (CTTC VIII), Cracow, Poland, September 1-4, 2019.

249.** "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," 20th International Conference on Recent Progress in Many-Body Theories, Toulouse, France, September 9-13, 2019.

250.** "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," The Utah Workshop on Quantum Methods in Molecular and Solid-State Theory, Park City, Utah, U.S.A., September 22-27, 2019.

251.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Workshop on New Methods for Strongly Correlated Electrons, Qingdao, China, October 9-13, 2019.

252.** "Introduction to the Single-Reference Many-Body Perturbation Theory and Its Diagrammatic Representation," Three-lecture mini-course given at the College of Chemistry and Molecular Engineering, Peking University, Beijing, China, November 12-14, 2019.

253.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," The Xingda Lectureship, College of Chemistry and Molecular Engineering, Peking University, Beijing, China, November 15, 2019.

254.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," The international conference "Quantum International Frontiers 2019," Shanghai, China, November 18-22, 2019 [invited Frontier Lecture].

255.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Department of Chemistry, North Carolina State University, Raleigh, North Carolina, U.S.A., January 20, 2020.

256.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," the 60th Sanibel Symposium, St. Simons Island, Georgia, U.S.A., February 16-21, 2020.

257.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Department of Physics, King's College London, London, U.K., March 3, 2020.

258.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Department of Chemistry, University of Cambridge, Cambdridge, U.K., March 4, 2020.

259.** "Toward Exact Quantum Chemistry," Computational Chemical Sciences Psi Group Zoom Meeting, April 15, 2020 [lecture via Zoom].

260.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Department of Chemistry, University of Chicago, May 1, 2020 [lecture via Zoom].

261.** "High-Accuracy Electronic Energetics by Stochastic and Deterministic Wave Function Sampling and Coupled-Cluster Computations," TSRC Workshop "Low-Scaling and Unconventional Electronic Structure Techniques" (LUEST 2020), 5th edition, Telluride, Colorado, U.S.A., June 1-5, 2020.
DUE TO COVID-19, REPLACED BY VIRTUAL WORKSHOP, June 1-5 and June 8-9, 2020 [lecture via Zoom].

262.** "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States (Toward Exact Quantum Chemistry)," 2020 Computational and Theoretical Chemistry Virtual Conference Series (July 16, July 30, August 13, 2020), Germantown, Maryland, U.S.A., August 13, 2020 [lecture via Zoom].

263.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Department of Chemistry, Purdue University, West Lafayette, Indiana, U.S.A., November 4, 2020 [lecture via Webex].

264.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Institute of Physics, Lódź University of Technology, Lódź, Poland, November 20, 2020 [lecture via Zoom].

265.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Seminar Series "Discussion on Many-Body Theory," CEA Saclay, France, November 27, 2020 [lecture via Zoom].

266.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," The Physical, Theoretical, and Computational Chemistry Virtual Seminar Series, Chemical Institute of Canada, December 1, 2020 [lecture via Zoom].

267.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Department of Chemistry, University of Florida, Gainesville, Florida, U.S.A., February 23, 2021 [lecture via Zoom].

268.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," School of Chemistry and Chemical Engineering, Nanjing University, Nanjing, China, April 8, 2021 [lecture via VooV].

269.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Department of Chemistry, University of Iowa, Iowa City, Iowa, U.S.A., April 16, 2021 [lecture via Zoom].

270.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," TSRC Workshop "New Frontiers in Electron Correlation," 3rd edition, Telluride, Colorado, U.S.A., June 14-18, 2021 [virtual workshop; lecture via Zoom].

271.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," The 4th TSRC Workshop "New Developments in Coupled-Cluster Theory," Telluride, Colorado, U.S.A., July 19-23, 2021 [hybrid format; lecture via Zoom].

272.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," International Symposium on Correlated Electrons (SymCorrel21), Munich Center for Quantum Science and Technology, Munich, Germany, October 5-7, 2021 [virtual workshop; lecture via Zoom].

273.** "Computational Studies of FR0-SB, a Novel Organic Compound that Deprotonates Alcohols upon Photoexcitation," International conference in the series "New Horizons in Scientific Software (NHISS 2021)" entitled "Light-Matter Interaction: Theory Meets Experiment," Jeju Island, South Korea, November 22-25, 2021 [hybrid format; lecture via Zoom].

274.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," The Seventeenth Theoretical Chemistry Symposium (TCS 2021), Indian Institute of Science Education and Research Kolkata, Mohanpur, Nadia, West Bengal, India, December 11-14, 2021 [virtual symposium; invited plenary lecture].

275.** "Externally Corrected Coupled-Cluster Methods Using Selected Configuration Interaction and FCIQMC," the 61st Sanibel Symposium, invited session on New Directions in

CC Theory, St. Simons Island, Georgia, U.S.A., February 13-18, 2022 [in-person invited plenary lecture].

276.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," Chris Cramer 60th Birthday Symposium, 263rd American Chemical Society National Meeting, San Diego, California, U.S.A., March 20-24, 2022 [in-person and virtual meeting; pre-recorded virtual presentation].

277.** "Recent Advances in Externally Corrected Coupled-Cluster Methods," 10th International Conference "Molecular Quantum Mechanics" entitled "Molecular Quantum Mechanics: Innovation, Impact, and Insight," in honor of Professors Gustavo Scuseria and Martin Head-Gordon, Blacksburg, Virginia, U.S.A., June 26 - July 1, 2022 [invited plenary lecture].

278.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," Twelfth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2020), Vancouver, British Columbia, Canada, August 16-21, 2020.
DUE TO COVID-19, RESCHEDULED TO July 3-8, 2022.

279.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," The 2020 American Conference on Theoretical Chemistry (ACTC 2020), Palisades Tahoe (formerly Squaw Valley), California, U.S.A., July 26-30, 2020.
DUE TO COVID-19, RESCHEDULED TO July 24-28, 2022; renamed ACTC 2022.

280.** "Recent Advances in Externally Corrected Coupled-Cluster Methods," The symposium "Quantum Chemistry: Current and Future Frontiers," 264th American Chemical Society National Meeting, Chicago, Illinois, U.S.A., August 21-25, 2022 [in-person and virtual meeting; in-person talk].

281.** "Recent Advances in Externally Corrected Coupled-Cluster Methods," OPERA-2020 (Operators, Perturbations, Electrons, Relativity, and Multi-Scale Applications), an international symposium on theoretical chemistry in honour of Prof. Jürgen Gauss on the occasion of his 60th birthday, Ingelheim am Rhein, Germany, September 1-3, 2021.
DUE TO COVID-19, RESCHEDULED TO August 31 - September 2, 2022.

282.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Faculty of Chemistry, University of Wrocław, Wrocław, Poland, September 7, 2022.

283.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Faculty of Chemistry, University of Warsaw, Warsaw, Poland, September 14, 2022.

284.** "Recent Advances in Externally Corrected Coupled-Cluster Methods," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Warsaw, Poland, September 15, 2022.

285.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Faculty of Chemistry, Jagiellonian University, Cracow, Poland, September 16, 2022.

286.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Modeling and Design of Molecular Materials 2020 (MDMM 2020) Conference, Gdańsk, Poland, September 21-24, 2020.
DUE TO COVID-19, RESCHEDULED TO September 19-22, 2022; renamed MDMM 2022.

287.** "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," International conference in the series "New Horizons in Scientific Software (NHISS 2022)" entitled "The New Collaborative Platform Goes Life," Jeju Island, South Korea, December 12-15, 2022 [hybrid format; lecture via Zoom].

288.** "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Department of Chemistry, Syracuse University, Syracuse, New York, U.S.A., January 31, 2023.

289.** "Computational Studies of FR0-SB, a Novel Organic Compound that Deprotonates Alcohols upon Photoexcitation," 28th Austin Symposium on Molecular Structure and Dynamics, Dallas, Texas, U.S.A., February 17-20, 2023.

290.** "Computational Studies of FR0-SB, a Novel Organic Compound that Deprotonates Alcohols upon Photoexcitation," J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic, June 19, 2023.

291.** "Externally Corrected Coupled-Cluster Methods: Review and Recent Progress," The symposium "Strong Correlation in Molecules," A Satellite Symposium to the 17th International Congress of Quantum Chemistry, Znojmo, Czech Republic.
DUE TO COVID-19, RESCHEDULED TO June 20-23, 2023 [special invited lecture during the session dedicated to the memory of Josef Paldus].

292.** "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches," 17th International Congress of Quantum Chemistry, Bratislava, Slovakia, June 21-26, 2021.
DUE TO COVID-19, RESCHEDULED TO June 26 - July 1, 2023 [invited plenary lecture].

293.** "Computational Studies of FR0-SB, a Novel Organic Compound that Deprotonates Alcohols upon Photoexcitation," The 41st Midwest Undergraduate Computational Chemistry Consortium (MU3C) Conference, Michigan State University, East Lansing, Michigan, U.S.A., August 1-2, 2023.

294.** "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches," The 5th Conference on Theory and Applications of Computational Chemistry (TACC 2020), Sapporo, Japan, September 7-12, 2020.
DUE TO COVID-19, RESCHEDULED TO September 4-9, 2023; renamed TACC 2023.

295.** "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches," 26th International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XXVI), Jaipur, Rajasthan, India, October 14-20, 2023 [hybrid format; lecture via Zoom].

296.** "Recent Progress in Externally Corrected Coupled-Cluster Methods: Following the Footsteps of a Legend (Lecture in Memory of Professor Josef Paldus)," The 37th Symposium on Chemical Physics at the University of Waterloo, Waterloo, Ontario, Canada, November 3-5, 2023 [special invited lecture in memory of Josef Paldus].

297.** "Quantum Chemistry and Physics," MSU Research Foundation Professorship Investiture Ceremony, Michigan State University, East Lansing, Michigan, U.S.A., November 14, 2023.

298.** "Addressing Strong Correlations Using Approximate Coupled-Pair Ideas: Following the Footsteps of a Legend (Lecture in Memory of Professor Josef Paldus)," the 63rd Sanibel Symposium, invited session on Coupled-Cluster Theory, St. Augustine Beach, Florida, U.S.A., February 25 - March 1, 2024 [invited plenary lecture].

299.** "Remembering Professor Josef Paldus: Pioneer of Modern Electronic Structure Theory and Caring Mentor, Educator, and Friend," Symposium "Advances in Electronic Structure Theory: A Symposium in Honour of Joe Paldus," the 107th Canadian Chemistry Conference and Exhibition (CSC 2024), Winnipeg, Manitoba, Canada, June 2-6, 2024.

300.** "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches," 30th Canadian Symposium on Theoretical and Computational Chemistry (CSTCC 2024), Halifax, Nova Scotia, Canada, July 21-25, 2024.

301.** "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches," The 5th TSRC Workshop "New Developments in Coupled-Cluster Theory," Telluride, Colorado, U.S.A., July 29 - August 2, 2024.

302.** "Converging High-Level Coupled-Cluster Energetics with Semi-Stochastic, CIPSI-Driven, and Adaptive CC(P;Q) Methods," 9th Conference "Current Trends in Theoretical Chemistry" (CTTC IX), Cracow, Poland, September 1-5, 2024.

303.** "Computational Studies of FR0-SB, a Novel Organic Compound that Deprotonates Alcohols upon Photoexcitation," Faculty of Chemistry, Jagiellonian University, Cracow, Poland, September 6, 2024.

304.** "Quantum Chemistry and Physics," MSU Research Foundation Board of Directors Meeting, Michigan State University, East Lansing, Michigan, U.S.A., September 20, 2024.

305.** "Converging High-Level Coupled-Cluster Energetics with Semi-Stochastic, CIPSI-Driven, and Adaptive CC(P;Q) Methods," Eleventh Congress of the International Society for Theoretical Chemical Physics (ISTCP-XI), symposium on Wave Function Theory for Electronic Structure, Qingdao, China, October 13-18, 2024.

306.** "Remembering Professor Josef Paldus: Pioneer of Modern Electronic Structure Theory and Caring Mentor, Educator, and Friend," Eleventh Congress of the International Society for Theoretical Chemical Physics (ISTCP-XI), Auqing Tang, Joe Paldus, and Bogumił Jeziorski Memorial Symposium and session on Chemical Insights, Qingdao, China, October 13-18, 2024.

307.** TBD, The symposium "Methods and Applications on Simulating Excited States: Molecular Dynamics, Spectroscopy, and Catalysis," 269th American Chemical Society National Meeting, San Diego, California, U.S.A., March 23-27, 2025.

308.** TBD, 11th Molecular Quantum Mechanics Conference (MQM 2025), in honor of Professors Hiroshi Nakatsuji and Kimihiko Hirao and in memory of Professors Keiji Morokuma and Shigeki Kato, Kyoto, Japan, May 23-28, 2025.

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

LIST OF PAPERS PRESENTED AT CONFERENCES[†]

1. P. Piecuch, "Invariance Properties of the Multipole Expansion," The Scientific Convention of the Polish Chemical Society and of the Association of Chemical Industry Engineers and Technicians, Lublin, Poland, September 22-25, 1982 [oral presentation].

2. P. Piecuch, "Spherical Tensor Operators in Theory of Long-Range Intermolecular Interactions," The Scientific Convention of the Polish Chemical Society and of the Association of Chemical Industry Engineers and Technicians, Lublin, Poland, September 22-25, 1982 [oral presentation].

3. P. Piecuch, "Spherical Tensor Theory of Long-Range Intermolecular Forces Including Quantum-Mechanical Many-Body Effects," Fourth School of Advanced Methods of Quantum Chemistry, Bachotek, Poland, May 27-31, 1985 [poster presentation].

4. P. Piecuch, "Simple Derivation of the Multipole Expansion in the Spherical Tensor Form. The Use of Stone's Cartesian-Spherical Transformation Formalism," Fourth School of Advanced Methods of Quantum Chemistry, Bachotek, Poland, May 27-31, 1985 [poster presentation].

5. P. Piecuch, "Mathematical Apparatus of the Quantum Theory of Angular Momentum and the Formalism of Irreducible Tensor Operators in the Perturbation Theory of Long-Range Interactions between N Molecules Including Many-Body Effects," Microsymposium of the Quantum Chemistry Section of the Polish Chemical Society organized during the Scientific Convention of the Polish Chemical Society and of the Association of Chemical Industry Engineers and Technicians, Poznań, Poland, September 4-7, 1985 [poster presentation].

6. P. Piecuch, "Magnitudes of Higher-Order Interaction Energy Contributions Appearing in the Perturbative Description of Long-Range Intermolecular Interactions. Interactions in the Typical Simple Molecular Complexes $H_2 - He$ and $H_2 - H_2$," Microsymposium of the Quantum Chemistry Section of the Polish Chemical Society organized during the Scientific Convention of the Polish Chemical Society and of the Association of Chemical Industry Engineers and Technicians, Poznań, Poland, September 4-7, 1985 [poster presentation].

7. P. Piecuch, "Anisotropic and Isotropic Two- and Many-Body Long-Range Intermolecular Interactions – the Use of Racah-Wigner Algebra and the Formalism of Irreducible Tensors," Conference "The Nature of Molecular Interactions," Karpacz, Poland, June 8-12, 1986 [poster presentation].

8. P. Piecuch, "Spherical Tensor Theory of Long-Range Molecular Interactions Including Quantum-Mechanical Many-Body Effects," International Symposium "Molecules in Physics, Chemistry and Biology," Paris, France, June 15-21, 1986 [poster presentation].

[†] Presentations of results that have been obtained at Michigan State University before submitting the tenure promotion package in the Fall of 2001 are marked by $*$. Presentations given after submitting the tenure promotion package in the Fall of 2001 are marked by $**$.

9. P. Piecuch, "Classification and Mathematical Description of Two- and Many-Body Long-Range Interactions in a System of N Arbitrary Molecules," Conference "Quantum Chemistry - 86," Wrocław, Poland, December 5-6, 1986 [oral presentation].

10. P. Piecuch, "Theoretical Insight into Many-Body Long-Range Effects of the Electrostatic Origin in Multimolecular Systems," 35. Bunsen-Kolloquium "Interactions of Water in Ionic and Nonionic Hydrates," Marburg, April 2-3, 1987 (and subsequent seminar of the Department of Physical Chemistry of the University of Marburg, April 4, 1987), Federal Republic of Germany [poster presentation].

11. P. Piecuch, "Elementary Derivation of the Addition Theorems for Solid Spherical Harmonics," Second School "Current Trends in Theoretical Chemistry," Zakopane, Poland, May 27-31, 1987 [poster presentation].

12. P. Piecuch, "Spherical Tensor Theory of Long-Range Intermolecular Forces Including Quantum-Mechanical Many-Body Effects: the Use of Cartesian-Spherical Transformation Formalism," Fifth School of Advanced Methods of Quantum Chemistry "Bachotek '87," Bachotek, Poland, May 31-June 5, 1987 [poster presentation].

13. P. Piecuch, "Analytical Description of Two- and Many-Body Fourth-Order Induction Interaction Energies in Multimolecular Systems within Spherical Tensor Formalism," Eighth International Symposium on Solute-Solute-Solvent Interactions, Regensburg, Federal Republic of Germany, August 9-14, 1987 [oral presentation].

14. P. Piecuch, "Classification and Analytical Description of Two- and Many-Body Fourth-Order Induction Interaction Energies in Multimolecular Systems within Spherical Tensor Formalism," VIII-th Workshop "Horizons in Hydrogen Bond Research," Polanica Zdrój near Wrocław, Poland, September 10-16, 1987 [poster presentation].

15. P. Piecuch, "Generalization of the Concept of Spherical Harmonic Expansions to Many-Body Intermolecular Forces. Application to the Case of Fourth-Order Induction Interactions in an Arbitrary Multimolecular System," Regional Symposium on Chemical Physics, University of Waterloo, Waterloo, Ontario, Canada, October 28-30, 1988 [poster presentation].

16. P. Piecuch and J. Paldus, "Orthogonally Spin-Adapted Coupled-Cluster Equations. Comparison of Different Procedures for Spin-Adaptation," Regional Symposium on Chemical Physics, University of Waterloo, Waterloo, Ontario, Canada, October 28-30, 1988 [poster presentation].

17. P. Piecuch, S. Zarrabian, J. Paldus, and J. Čížek, "Coupled-Cluster Approach with Approximate Account of Triple Excitations and its Application to the Cyclic Polyene Model Systems," 10th Canadian Symposium on Theoretical Chemistry, Banff, Alberta, Canada, August 24-30, 1989 [poster presentation].

18. P. Piecuch, S. Zarrabian, J. Paldus, and J. Čížek, "Limitations in Determining the Lower Bounds to the Ground State Correlation Energy of the Cyclic Polyenes Using Optimized Inner Projection Technique," 10th Canadian Symposium on Theoretical Chemistry, Banff, Alberta, Canada, August 24-30, 1989 [poster presentation].

19. P. Piecuch, S. Zarrabian, J. Paldus, and J. Čížek, "Account of Higher than Pair Cluster Contributions in Single Reference Coupled Cluster Theory," The 6^{th} Annual University of Waterloo Symposium on Chemical Physics, University of Waterloo, Waterloo, Ontario, Canada, October 26-28, 1990 [poster presentation].

20. P. Piecuch and J. Paldus, "Orthogonally Spin-Adapted Multi-Reference Coupled-Cluster Formalism. Comparison of Different Procedures for Spin-Adaptation," 1991 Sanibel Symposia on Atomic, Molecular, and Condensed Matter Theory, Computational Methods, and the Application of Fundamental Theory to Problems of Biology and Pharmacology, St. Augustine, Florida, U.S.A., March 9-16, 1991 [poster presentation].

21. J. Paldus, P. Piecuch, B. Jeziorski, and L. Pylypow, "Extension of Coupled Cluster Methodology to Open Shells: State-Universal Approach," Seventh International Conference on Recent Progress in Many-Body Theories, Minneapolis, Minnesota, U.S.A., August 26-31, 1991 [invited talk given by J. Paldus].

22. P. Piecuch, R. Toboła, J. Paldus, and H. Chojnacki, "Approximate Method of Accounting for Quadruple Excitations in Multi-Reference Coupled-Cluster Theory. Application to H_4 Model System," Quantum Chemistry Symposium on Methods and Applications of Quantum Chemistry in Studies of Molecular Systems organized by the Institute of Chemistry of the Silesian University in cooperation with Quantum Chemistry Section of the Polish Chemical Society, Katowice, Poland, September 18, 1992 [poster presentation].

23. P. Piecuch, "Application of the Hilbert-Space Coupled-Cluster Theory to Electronic States of the H_4 Model System," Workshop "Coupled Clusters in the Theory of Atoms and Molecules," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Poland, October 23-24, 1992 [invited talk].

24. J. Paldus, X. Li, and P. Piecuch, "Degeneracy and Coupled-Cluster Methods ('Variations on a Theme')," 1993 Sanibel Symposia on Atomic, Molecular, and Condensed Matter Theory, Computational Methods, and the Application of Fundamental Theory to Problems of Biology and Pharmacology, St. Augustine, Florida, U.S.A., March 13-20, 1993 [poster presentation].

25. J. Paldus and P. Piecuch, "Exclusion Principle Violating (EPV) Diagrams: A Mathematical Convenience or a Physically Important Concept?," 5th International Conference on Mathematical and Computational Chemistry, University of Missouri-Kansas City, Kansas City, Missouri, U.S.A., May 17-21, 1993 [talk given by J. Paldus].

26. P. Piecuch and L. Adamowicz, "A State-Selective Multi-Reference Coupled-Cluster Method Employing the Single-Reference Formalism: Theory, Implementation and a Test Case Study," 14th Annual West Coast Theoretical Chemistry/Statistical Mechanics Conference, University of California, Los Angeles, California, U.S.A., June 17-19, 1993 [contributed talk given by P. Piecuch].

27. P. Piecuch and L. Adamowicz, "A State-Selective Multi-Reference Coupled-Cluster Method Employing the Single-Reference Formalism: Theory, Implementation and a Model Study," Eighth American Conference on Theoretical Chemistry, University of Rochester, Rochester, New York, U.S.A., June 27-July 2, 1993 [poster presentation].

28. P. Piecuch and L. Adamowicz, "Breaking Bonds with the SS MRCC Method," 15th Annual West Coast Theoretical Chemistry/Statistical Mechanics Conference, Sandia National Laboratories, Livermore, California, U.S.A., April 27-29, 1994 [poster presentation].

29. V. Alexandrov, P. Piecuch, and L. Adamowicz, "State-Selective Multireference Coupled-Cluster Theory Employing Single-Reference Formalism: Implementation and Application to Excited States of LiH and H_8," 15th Annual West Coast Theoretical Chemistry/Statistical Mechanics Conference, Sandia National Laboratories, Livermore, California, U.S.A., April 27-29, 1994 [contributed talk given by V. Alexandrov].

30. P. Piecuch and J. Paldus, "Orthogonally Spin-Adapted Hilbert-Space Coupled-Cluster Formalism. Importance of the High-Order Coupling Terms," Second Canadian Computational Chemistry Conference, Queen's University at Kingston, Kingston, Ontario, Canada, May 21-25, 1994 [plenary talk given by P. Piecuch].

31. P. Piecuch, V. Alexandrov, and L. Adamowicz, "A State-Selective Multi-Reference Coupled-Cluster Method Employing the Single-Reference Formalism: Theory, Implementation and a Model Study," 8th International Congress of Quantum Chemistry, Satellite Meeting "Electron Correlation in Atoms and Molecules; New Methods and Applications," Smolenice Castle near Bratislava, Slovak Republic, June 14-18, 1994 [talk given by L. Adamowicz].

32. R. Toboła, P. Piecuch, and J. Paldus, "Coupled Cluster Approaches with an Approximate Account of Triply and Quadruply Excited Clusters: Implementation of the Orthogonally Spin-Adapted CCD+ST(CCD), CCSD+T(CCSD) and ACPQ+ST(ACPQ) Formalisms," 8th International Congress of Quantum Chemistry, Satellite Meeting "Electron Correlation in Atoms and Molecules; New Methods and Applications," Smolenice Castle near Bratislava, Slovak Republic, June 14-18, 1994 [poster presentation].

33. R. Toboła, P. Piecuch, J. Paldus, and H. Chojnacki, "Coupled Cluster Approaches with an Approximate Account of Triply and Quadruply Excited Clusters: Implementation of the Orthogonally Spin-Adapted CCD+ST(CCD) and ACPQ+ST(ACPQ) Formalisms," The Scientific Convention of the Polish Chemical Society and of the Association of Chemical Industry Engineers and Technicians, Warsaw, Poland, September 12-15, 1994 [poster presentation].

34. P. Piecuch and J. Paldus, "Coupled-Cluster Methods for Quasidegenerate States. Calculation of Potential Energy Surfaces and Molecular Properties Using the State-Universal Multi-Reference Coupled-Cluster Approach," The 10^{th} Annual University of Waterloo Symposium on Chemical Physics, University of Waterloo, Waterloo, Ontario, Canada, November 4-6, 1994 [plenary talk given by P. Piecuch].

35. A.E. Kondo, P. Piecuch, and J. Paldus, "Orthogonally Spin-Adapted Single-Reference Coupled-Cluster Formalism: Linear Response Calculation of Static Properties," The 10^{th} Annual University of Waterloo Symposium on Chemical Physics, University of Waterloo, Waterloo, Ontario, Canada, November 4-6, 1994 [poster presentation].

36. P. Piecuch, A.E. Kondo, V. Špirko, and J. Paldus, "Calculation of Property Functions Using the Single- and Multi-Reference Coupled-Cluster Approaches," 12th Canadian

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

37. J. Paldus, X. Li, and P. Piecuch, "Recent Developments in Coupled-Cluster Theory," 1995 International Chemical Congress of Pacific Basin Societies (PACIFICHEM '95), Honolulu, Hawaii, U.S.A., December 17-22, 1995 [invited talk given by J. Paldus].

38. J. Paldus, P. Piecuch, X. Li, and A.E. Kondo, "Coupled Cluster Approach to Static Properties," Canadian Society for Chemistry, 79th Conference and Exhibition, Memorial University of Newfoundland, St. John's, Canada, June 23-26, 1996 [invited talk given by J. Paldus].

39. P. Piecuch, A.E. Kondo, J. Paldus, and V. Špirko, "Linear Response Coupled-Cluster Approach to Static Molecular Properties," The symposium "Frontiers in Electronic Structure Theory," 213th American Chemical Society National Meeting, San Francisco, California, U.S.A., April 13-17, 1997 [invited talk given by P. Piecuch].

40. P. Piecuch, "Coupled-Cluster Approach to Static Molecular Properties," Workshop "Coupled Cluster Theory and Electron Correlation, Fifty Years of the Correlation Problem," Cedar Key, Florida, U.S.A., June 15-19, 1997, a satellite meeting of the 9th International Congress of Quantum Chemistry, Atlanta, Georgia, U.S.A., June 9-14, 1997 [invited talk].

41. M.S. Topaler, D.G. Truhlar, X.Y. Chang, P. Piecuch, and J.C. Polanyi, "Fit of Potential Energy Surfaces and Theoretical Study of NaFH Absorption and Photodissociation Cross Sections," 1997 Conference on the Dynamics of Molecular Collisions, Gull Lake, Minnesota, U.S.A., July 21-25, 1997 [poster presentation].

42. P. Piecuch and R.J. Bartlett, "EOMXCC: A New Coupled-Cluster Method for Electronically Excited States," Thirty-Eighth Sanibel Symposium on Atomic, Molecular, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 21-27, 1998 [poster presentation].

43. P. Piecuch, S.A. Kucharski, and R.J. Bartlett, "Coupled-Cluster Methods with Internal and Semi-Internal Triply and Quadruply Excited Clusters: CCSDt and CCSDtq Approaches," Twenty-Seventh Southeastern Theoretical Chemistry Association Conference, Tallahassee, Florida, U.S.A., May 28-30, 1998 [contributed talk given by P. Piecuch].

44.* V. Špirko, P. Piecuch, and O. Bludsky, "Quasi-Bound States of the Na$\cdots$FH van der Waals Molecule," Thirty-Ninth Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 27-March 5, 1999 [poster presentation].

45.* S.A. Kucharski, P. Piecuch, and R.J. Bartlett, "Potential Energy Curves for the N_2 Molecule: A Coupled Cluster Study Including Connected Quadruply Excited Clusters," Thirty-Ninth Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 27-March 5, 1999 [poster presentation].

46.* P. Piecuch, "Single-Reference Coupled-Cluster Methods for Quasi-Degenerate Electronic States," The symposium "Electronic Structure Theory: From Methods to Molecules and Materials," 100th Annual Meeting of the American Physical Society, Atlanta, Georgia, U.S.A., March 21-26, 1999 [invited talk].

47.* J.B. Giorgi, T.G. Lee, A.J. Hudson, F. Naumkin, H.-B. Oh, P. Piecuch, and J.C. Polanyi, "Harpooning Studied by Transition-State Spectroscopy: $M \cdot\cdot XR + h\nu \rightarrow [M^* \cdot\cdot XR]^\ddagger \rightarrow [M^+ \cdots XR^-]^\ddagger \rightarrow$ products ($X = F, Cl, Br$; $R = H, CH_3$)," The symposium "Electronically Nonadiabatic Processes in Gaseous, Cluster, and Condensed Media," 218th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., August 22-26, 1999 [invited talk given by J.C. Polanyi].

48.* P. Piecuch, "Dynamics of Harpooning in van der Waals Molecules," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999 [invited talk].

49.* K. Kowalski and P. Piecuch, "On the Origin of Intruder State Problem in Multi-Reference Coupled-Cluster Theory," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999 [poster presentation].

50.* K. Kowalski, P. Piecuch, and K. Jankowski, "A Complete Set of Solutions of Coupled-Cluster Equations Involving Triply and Quadruply Excited Clusters," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999 [poster presentation].

51.* P. Piecuch and J.I. Landman, "Parallelization of Multi-Reference Coupled-Cluster Method," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999 [poster presentation].

52.* P. Piecuch, S.A. Kucharski, and V. Špirko, "Coupled-Cluster Methods with Internal and Semi-Internal Triply Excited Clusters: Vibrational Spectrum of the HF Molecule," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999 [poster presentation].

53.* R.J. Bartlett, S.A. Kucharski, P. Piecuch, K. Wilson, M. Kolaski, and S.A. Perera, "Coupled-Cluster Theory: Recent Progress," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999 [invited talk given by R.J. Bartlett].

54.* P. Piecuch, "Dynamics of Harpooning in van der Waals Molecules," "Vth International Conference on Molecular Spectroscopy," Lądek-Zdrój, Poland, September 26-30, 1999 [invited talk].

55.* P. Piecuch and K. Kowalski, "Method of Moments of Coupled Cluster Equations: A New Approach to the Many-Electron Correlation Problem," 40th Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 26-March 3, 2000 [poster presentation].

56.* K. Kowalski and P. Piecuch, "The Complete Sets of Solutions of the Bloch and State-Universal Multi-Reference Coupled-Cluster Equations," 40th Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 26-March 3, 2000 [poster presentation].

57.* R. Burcl, P. Piecuch, V. Špirko, and O. Bludský, "Bound and Quasi-Bound States of the $Li\cdots FH$ van der Waals Molecule," 40th Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 26-March 3, 2000 [poster presentation].

58.* J.B. Giorgi, T.G. Lee, A.J. Hudson, F. Naumkin, H.-B. Oh, P. Piecuch, and J.C. Polanyi, "Harpooning Studied by Transition-State Spectroscopy: $M\cdot\cdot XR + h\nu \rightarrow [M^*\cdot\cdot XR]^\ddagger \rightarrow [M^+\cdots XR^-]^\ddagger \rightarrow$ products: Results for $M = Li$, $X = F$, $R = H, CH_3$," The symposium "Computers in Chemistry Award Symposium Honoring Don Truhlar," 219th American Chemical Society National Meeting, San Francisco, California, U.S.A., March 26-30, 2000 [invited talk given by J.C. Polanyi].

59.* P. Piecuch and K. Kowalski, "Method of Moments of Coupled-Cluster Equations: A New Approach to the Many-Electron Correlation Problem," The 2000 Florida Award Symposium (honoring Dr. Rodney J. Bartlett's work), FAME 2000 (Florida Annual Meeting and Exposition, organized by the Florida Section of the American Chemical Society), Orlando, Florida, U.S.A., May 12, 2000 [invited talk given by P. Piecuch].

60.* P. Piecuch, "Dynamics of Photo-Induced Charge Transfer in van der Waals Molecules," Joint Polish-German Conference on Modern Optics: Fundamental Aspects of Spectroscopy and Environmental Applications, Jurata near Gdańsk, Poland, September 17-22, 2000 [invited talk].

61.* R. Burcl, P. Piecuch, V. Špirko, and O. Bludsky, "Bound and Quasi-Bound States of the $Li\cdots FH$ van der Waals Molecule," The 16th Annual Symposium on Chemical Physics at the University of Waterloo, Waterloo, Ontario, Canada, November 3-5, 2000 [contributed talk, given by R. Burcl].

62.* E. Kratz, R. Burcl, P. Piecuch, and V. Špirko, "*Ab Initio* Studies of the $Li\cdots FCH_3$ van der Waals Complex," The 16th Annual Symposium on Chemical Physics at the University of Waterloo, Waterloo, Ontario, Canada, November 3-5, 2000 [poster presented by R. Burcl].

63.* P. Piecuch, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," the 41st Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 24-March 2, 2001 [invited talk].

64.* K. Kowalski and P. Piecuch, "New Equation-of-Motion Coupled-Cluster Methods," the 41st Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 24 - March 2, 2001 [poster, presented by K. Kowalski].

65.* P. Piecuch, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," First Southern School on Computational Chemistry, Orange Beach, Alabama, March 24, 2001 [invited talk].

66.* P. Piecuch and K. Kowalski, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," 14th Canadian Symposium on Theoretical Chemistry, Carleton University, Ottawa, Canada, August 4-9, 2001 [contributed talk given by P. Piecuch; one of the three posters selected for oral presentations].

67.* P. Piecuch, V. Špirko, R. Burcl, K. Kowalski, S.A. Kucharski, F. Mrugała, and O. Bludsky, "Effect of the Potential Energy Surface on the Dynamics of Weakly Bound Precursor Complexes and New "Black-Blox" Coupled-Cluster Methods for Entire Potential Energy Surfaces of Reactive Molecular Systems," The symposium "First Principles Chemical Reaction Dynamics," 222nd American Chemical Society National Meeting, Chicago, Illinois, U.S.A., August 26-30, 2001 [invited talk given by P. Piecuch].

68.* P. Piecuch, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," 34th Midwest Theoretical Chemistry Conference, University of Minnesota, Minneapolis, Minnesota, U.S.A., October 5-6, 2001 [invited talk].

69.* K. Kowalski and P. Piecuch, "New Equation-of-Motion Coupled-Cluster Methods," 34th Midwest Theoretical Chemistry Conference, University of Minnesota, Minneapolis, Minnesota, U.S.A., October 5-6, 2001 [poster presented by K. Kowalski].

70.* A.W. Jasper, M.D. Hack A. Chakraborty, P. Piecuch, and D.G. Truhlar, "Photodissociation of LiFH and NaFH van der Waals Complexes: A Semiclassical Trajectory Study," 34th Midwest Theoretical Chemistry Conference, University of Minnesota, Minneapolis, Minnesota, U.S.A., October 5-6, 2001 [poster presented by A.W. Jasper].

71.* P. Piecuch, K. Kowalski, and I.S.O. Pimienta, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," the 262nd WE-Heraeus-Seminar entitled "Modern Aspects of Many-Electron Theory," Bad Honnef, Germany, October 21-24, 2001 [invited poster, presented by P. Piecuch].

72.** K. Kowalski and P. Piecuch, "New Coupled-Cluster Methods for Excited States," 10th Conference on Current Trends in Computational Chemistry, Jackson, Missisipi, U.S.A., November 1-3, 2001 [poster presented by K. Kowalski].

73.** P. Piecuch, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces: I. Ground-State Approaches," SciDAC Kick-Off Meeting, Reston, Virginia, U.S.A., January 15-16, 2002 [poster].

74.** P. Piecuch, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces: II. Excited-State Approaches," SciDAC Kick-Off Meeting, Reston, Virginia, U.S.A., January 15-16, 2002 [poster].

75.** P. Piecuch, "Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Quasi-Degenerate Ground States, Molecular Potential Energy Surfaces, and Excited States," Institute for Nuclear Theory workshop on "Advanced Computational Methods for Solving the Nuclear Many-Body Problem," Seattle, Washington, U.S.A., March 12-15, 2002 [invited talk].

76.** P. Piecuch, K. Kowalski, and I.S.O. Pimienta, "New Single- and Multi-Reference Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," The

symposium "Recent Advances in Electron Correlation Methodology," 223rd American Chemical Society National Meeting, Orlando, Florida, U.S.A., April 7-11, 2002 [invited talk given by P. Piecuch].

77.** P. Piecuch, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces: Recent Progress and Milestones," BES SciDAC PI Workshop, Argonne National Laboratory, Argonne, Illinois, U.S.A., June 13-14, 2002 [poster].

78.** I.S.O. Pimienta, K. Kowalski, and P. Piecuch, "Method of Moments of Coupled-Cluster Equations: Inclusion of All Generalized Moments of the Coupled-Cluster Singles and Doubles Equations," The 2002 American Conference on Theoretical Chemistry, Seven Springs Mountain Resort, Champion, Pennsylvania, U.S.A., July 13-18, 2002 [poster presented by I.S.O. Pimienta].

79.** K. Kowalski and P. Piecuch, "New Equation-of-Motion Coupled-Cluster Methods," The 2002 American Conference on Theoretical Chemistry, Seven Springs Mountain Resort, Champion, Pennsylvania, U.S.A., July 13-18, 2002 [poster presented by K. Kowalski].

80.** M.J. McGuire, E. Kratz, R. Burcl, and P. Piecuch, "The Unusual Effect of the Basis Set Superposition Error on the Geometries and Bending Potentials of the $Li \cdots FCH_3$ and $Na \cdots FCH_3$ Complexes," The 2002 American Conference on Theoretical Chemistry, Seven Springs Mountain Resort, Champion, Pennsylvania, U.S.A., July 13-18, 2002 [poster presented by M.J. McGuire].

81.** M.J. McGuire, K. Kowalski, and P. Piecuch, "Renormalized Coupled-Cluster Calculations of Reactive Potential Energy Surfaces: The Collinear BeFH System," The 2002 American Conference on Theoretical Chemistry, Seven Springs Mountain Resort, Champion, Pennsylvania, U.S.A., July 13-18, 2002 [poster presented by M.J. McGuire].

82.** P.-D. Fan, K. Jedziniak, K. Kowalski, and P. Piecuch, "On the Exactness of Two-Body Cluster Expansions in Many-Body Quantum Theory," The 2002 American Conference on Theoretical Chemistry, Seven Springs Mountain Resort, Champion, Pennsylvania, U.S.A., July 13-18, 2002 [poster presented by P.-D. Fan].

83.** P. Piecuch, K. Kowalski, I.S.O. Pimienta, and M.J. McGuire, "Method of Moments of Coupled-Cluster Equations: A New Framework for Designing Accurate Electronic Structure Methods," Fourth International Congress of the International Society for Theoretical Chemical Physics (ICTCP-IV), Marly-le-Roi near Paris, France, July 9-16, 2002 [invited plenary talk given by P. Piecuch].

84.** P. Piecuch, "Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing Highly Accurate Electronic Structure Methods," International Symposium on Frontiers in Molecular Science 2002, Qingdao, China, July 15-18, 2002 [invited talk].

85.** P. Piecuch, K. Kowalski, and I.S.O. Pimienta, "Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," 6th World Congress of Theoretically Oriented Chemists (WATOC02), Lugano, Switzerland, August 4-9, 2002 [contributed talk; paper selected by the Organizers for the oral presentation].

86.** P. Piecuch, K. Kowalski, I.S.O. Pimienta, M.J. McGuire, and P.-D. Fan, "Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing Highly Accurate (Virtually Exact) and Inexpensive Electronic Structure Methods," 11th Conference on Current Trends in Computational Chemistry, Jackson, Missisipi, U.S.A., November 1-2, 2002 [invited talk given by P. Piecuch].

87.** I.S.O. Pimienta, P. Piecuch, and K. Kowalski, "Method of Moments of Coupled-Cluster Equations: Inclusion of All Generalized Moments of the Coupled-Cluster Singles and Doubles Equations," the 43rd Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 22-March 1, 2003 [poster, presented by I.S.O. Pimienta].

88.** P.-D. Fan, K. Kowalski, and P. Piecuch, "New Alternatives for Electronic Structure Theory: The Applications of Two-Body Cluster Expansions in Accurate *Ab Initio* Calculations," the 43rd Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 22-March 1, 2003 [poster, presented by P.-D. Fan].

89.** P. Piecuch, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," 2003 DOE SciDAC PI Meeting, Napa, California, U.S.A., March 10-11, 2003 [poster].

90.** P. Piecuch, K. Kowalski, I.S.O. Pimienta, and P.-D. Fan, "New Alternatives for Accurate Electronic Structure Calculations of Molecular Potential Energy Surfaces," The symposium "New Electronic Structure Methods: From Molecules to Materials," 225th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., March 23-27, 2003 [invited talk given by P. Piecuch].

91.** P. Piecuch, K. Kowalski, P.-D. Fan, and K. Jedziniak, "On the Exactness of Two-Body Cluster Expansions in Many-Body Quantum Theory," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12-14, 2003 [talk given by P. Piecuch].

92.** K. Kowalski and P. Piecuch, "A New Class of Noniterative Energy Corrections to Coupled-Cluster Energies for Excited Electronic States," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12-14, 2003 [talk given by K. Kowalski].

93.** M.J. McGuire, P. Piecuch, K. Kowalski, S.A. Kucharski, and M. Musiał, "Renormalized Coupled-Cluster Calculations of Reactive Potential Energy Surfaces: A Comparison of the CCSD(T), Renormalized CCSD(T), and Multi-Reference Configuration Interaction Results for the BeFH System," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12-14, 2003 [poster presented by M.J. McGuire].

94.** M.J. McGuire, E. Kratz, R. Burcl, and P. Piecuch, "The Unusual Effect of the Basis Set Superposition Error on the Geometries and Bending Potentials of the Li$\cdots$FCH$_3$ and Na$\cdots$FC H$_3$ Complexes," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12-14, 2003 [talk given by M.J. McGuire].

95.** I.S.O. Pimienta, Piotr Piecuch, and K. Kowalski, "Method of Moments of Coupled-Cluster Equations: Inclusion of All Generalized Moments of the Coupled-Cluster Singles and Doubles Equations," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12-14, 2003 [talk given by I.S.O. Pimienta].

96.** P.-D. Fan, K. Kowalski, and P. Piecuch, "The Application of the Extended Coupled-Cluster Method with Singles and Doubles in Studies of Bond Breaking," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12-14, 2003 [talk given by P.-D. Fan].

97.** M. Lodriguito, P.-D. Fan, K. Kowalski, and P. Piecuch, " Method of Moments of Coupled-Cluster Equations Employing the Extended Coupled-Cluster Theory: Dissociation of the N_2 Triple Bond," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12-14, 2003 [poster presented by M. Lodriguito].

98.** R.C. Lafuente, P. Piecuch, and K.L.C. Hunt, "Towards the Development and Implementation of Computer Programs for Calculating the Charge-Density Susceptibility," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12-14, 2003 [poster presented by R.C. Lafuente].

99.** R.M. Olson, S.A. Varganov, M.S. Gordon, G. Mill, H. Metiu, and P. Piecuch, "2D/3D Transition of Small Gold Clusters ($Au_n|n = 4, 6, 8, \ldots$)," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12-14, 2003 [poster presented by R.M. Olson].

100.** P. Piecuch, K. Kowalski, I.S.O. Pimienta, P.-D. Fan, and M.J. McGuire, "Single- and Multi-reference Coupled-Cluster Methods for Quasidegenerate Electronic States and Bond Breaking," The symposium "Bond-Breaking Methods in Gas and Condensed Phases," 226th American Chemical Society National Meeting, New York, New York, U.S.A., September 7-11, 2003 [invited talk given by P. Piecuch].

101.** K. Kowalski and P. Piecuch, "A New Class of Noniterative Energy Corrections to Coupled-Cluster Energies for Excited Electronic States," The symposium "Bond-Breaking Methods in Gas and Condensed Phases," 226th American Chemical Society National Meeting, New York, New York, U.S.A., September 7-11, 2003 [talk given by K. Kowalski].

102.** T. Kuś, S.A. Kucharski, M.J. McGuire, K. Kowalski, and P. Piecuch, "Potential Energy Curves of Open-Shell Systems Obtained with Coupled-Cluster Methods with the T_3 Operator," The 46th Meeting of the Polish Chemical Society, Lublin, Poland, September 15-19, 2003 [poster presented by T. Kuś].

103.** P.-D. Fan, K. Kowalski, M. Lodriguito, and P. Piecuch, "New Alternatives for Accurate *Ab Initio* Calculations," 12th Conference on Current Trends in Computational Chemistry, Jackson, Missisipi, U.S.A., October 31-November 1, 2003 [poster presented by P.-D. Fan].

104.** P. Piecuch, "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States," 2004 DOE SciDAC PI Meeting, Charleston, South Carolina, U.S.A., March 22-24, 2004 [poster].

105.** P. Piecuch and K. Kowalski, "Noniterative Coupled-Cluster Methods for Accurate Calculations of Excited Electronic States," The symposium "The Systematic Treatment of Electron Correlation. A Celebration of the Science of Rodney J. Bartlett," St. Simons Island, Georgia, U.S.A., April 23-25, 2004 [invited talk given by P. Piecuch].

106.** D.J. Dean, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock, and P. Piecuch, "Coupled-Cluster Approaches to Nuclei, Ground States and Excited States," 8th International Spring Seminar on Nuclear Physics, Key Topics in Nuclear Structure, Paestum, Italy, May 23-27, 2004 [invited talk given by M. Hjorth-Jensen].

107.** P.-D. Fan, K. Kowalski, and P. Piecuch, "Intriguing Accuracy of Two-Body Cluster Expansions of Ground and Excited States," 36th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 17-19, 2004 [poster presented by P.-D. Fan].

108.** K. Kowalski and P. Piecuch, "New Classes of Noniterative Energy Corrections to Multireference Coupled-Cluster Energies," 36th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 17-19, 2004 [poster presented by K. Kowalski].

109.** R.C. Lafuente, K.L.C. Hunt, and P. Piecuch, "Preliminary Development and Implementation of Computer Programs for Calculating the Charge-Density Susceptibility," 36th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 17-19, 2004 [poster presented by R.C. Lafuente].

110.** M. Lodriguito, K. Kowalski, and P. Piecuch, "Method of Moments of Coupled-Cluster Equations Employing the Multireference Perturbation Theory," 36th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 17-19, 2004 [poster presented by M. Lodriguito].

111.** M.J. McGuire and P. Piecuch, "Application of Renormalized Coupled-Cluster Methods to Reactions Involving Diradicals," 36th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 17-19, 2004 [poster presented by M.J. McGuire].

112.** K. Kowalski, M. Włoch, and P. Piecuch, "Efficient Implementation of the Standard and Renormalized Equation-of-Motion Coupled-Cluster Methods in GAMESS," 36th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 17-19, 2004 [poster presented by M. Włoch].

113.** D.J. Dean, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock, and P. Piecuch, "Coupled-Cluster Approaches to Nuclei, Ground States and Excited States," International Nuclear Physics Conference, INPC 2004, Göteborg, Sweden, June 27-July 2, 2004 [invited talk given by M. Hjorth-Jensen].

114.** P. Piecuch, "Coupled-Cluster Method: An Accurate Ab Initio Theory of Atoms, Molecules, Nuclei, and Other Many-Fermion Systems," International Workshop on Microscopic Approaches to Nuclear Structure Calculations," UMIST, Manchester, U.K., July 4-8, 2004 [invited talk given by P. Piecuch].

115.** P. Piecuch, "Coupled-Cluster Approaches to Atoms, Molecules, and Nuclei," Workshop "New Perspectives on p-Shell Nuclei," Michigan State University, East Lansing, Michigan, U.S.A., July 22-24, 2004 [invited talk given by P. Piecuch].

116.** P. Piecuch, K. Kowalski, I.S.O. Pimienta, M. J. McGuire, P.-D. Fan, and M. Lodriguito, "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States," International conference "Molecular Quantum Mechanics: the No Nonsense Path to Progress" honoring Professor Nicholas Handy's work, St. John's College, Cambridge University, Cambridge, U.K., July 24-29, 2004 [invited talk given by P. Piecuch].

117.** P. Piecuch, P.-D. Fan, S. Hirata, and K. Kowalski, "Renormalized Coupled-Cluster Methods and their Automated Parallel Computer Implementation with Tensor Contraction Engine," The symposium "Symbolic Calculation in Chemistry," 228th American Chemical Society National Meeting, Philadelphia, Pennsylvania, U.S.A., August 22-26, 2004 [invited talk given by P. Piecuch].

118.** P. Piecuch, K. Kowalski, D.J. Dean, M. Hjorth-Jensen, T. Papenbrock, and M. Włoch, "Coupled Cluster Calculations of Ground and Excited States of Nuclei," International Conference on Exotic Nuclei and Atomic Masses, ENAM-04, Pine Mountain, Georgia, U.S.A., September 12-16, 2004 [invited contributed talk given by P. Piecuch].

119.** P. Piecuch, K. Kowalski, M. Włoch, and M. Lodriguito, "Non-Iterative Coupled-Cluster Methods For Accurate Calculations of Excited Electronic States," Ninth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-IX, Les Houches, Grenoble, France, September 25-30, 2004 [invited talk given by P. Piecuch].

120.** P. Piecuch, M. Włoch, D.J. Dean, J.R. Gour, M. Hjorth-Jensen, K. Kowalski, and T. Papenbrock, "Coupled Cluster Calculations of Ground and Excited States of Nuclei," Ninth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-IX, Les Houches, Grenoble, France, September 25-30, 2004 [invited talk given by P. Piecuch].

121.** P. Piecuch, "Coupled-Cluster Approaches to Atoms, Molecules, and Nuclei," Institute for Nuclear Theory workshop "Microscopic Nuclear Structure Theory," "Nuclear Forces and the Quantum Many-Body Problem," Seattle, Washington, U.S.A., October 4-8, 2004 [invited talk given by P. Piecuch].

122.** M.D. Lodriguito, K. Kowalski, and P. Piecuch, "Method of Moments of Coupled-Cluster Equations Employing the Multireference Perturbation Theory," The symposium "Computational Chemical Dynamics from Gas-Phase to Condensed-Phase Systems," Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, U.S.A., October 7-9, 2004 [poster presented by M. Lodriguito].

123.** P. Piecuch, "Coupled-Cluster Method: Highly Accurate Microscopic Approach to Molecular Systems and Nuclei," Workshop "Nuclei and Mesoscopic Physics," Michigan State University, East Lansing, Michigan, U.S.A., October 23-26, 2004 [invited talk given by P. Piecuch].

124.** P. Piecuch, K. Kowalski, M. Włoch, J.R. Gour, M.J. McGuire, P.-D. Fan, A. Kinal, and M. Lodriguito, "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals,

and Excited Electronic States," 7th World Congress of Theoretically Oriented Chemists (WATOC05), Cape Town, South Africa, January 16-21, 2005. [invited talk given by P. Piecuch].

125.** D.J. Dean, J.R. Gour, G. Hagen, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock, P. Piecuch, and M. Włoch, "Challenges for Nuclear Structure: From Stable to Weakly Bound Nuclei," International Symposium on Correlation Dynamics in Nuclei – on the Occasion of the 50th Anniversary of the Configuration Mixing Theory of Arima and Horie, CDN05, Tokyo, Japan, January 31-February 4, 2005 [invited talk given by M. Hjorth-Jensen].

126.** M.J. McGuire and P. Piecuch, "Renormalized Coupled-Cluster Studies of Reactions Involving Diradicals," the 45th Sanibel Symposium on Forefront Theory and Computation in Quantum Chemistry, Condensed Matter and Chemical Physics, Nanoscience, Quantum Biochemistry and Biophysics," St. Simons Island, Georgia, U.S.A., March 5-11, 2005 [poster presented by M.J. McGuire].

127.** A. Kinal and P. Piecuch, "Is the Mechanism of Cycloaddition of Ethylene to Cyclopentyne Concerted or Biradical? A Completely Renormalized Coupled Cluster Study," the 45th Sanibel Symposium on Forefront Theory and Computation in Quantum Chemistry, Condensed Matter and Chemical Physics, Nanoscience, Quantum Biochemistry and Biophysics," St. Simons Island, Georgia, U.S.A., March 5-11, 2005 [poster presented by A. Kinal].

128.** M.D. Lodriguito, K. Kowalski, M. Włoch, and P. Piecuch, "Method of Moments of Coupled-Cluster Equations Employing the Multireference Perturbation Theory," the 45th Sanibel Symposium on Forefront Theory and Computation in Quantum Chemistry, Condensed Matter and Chemical Physics, Nanoscience, Quantum Biochemistry and Biophysics," St. Simons Island, Georgia, U.S.A., March 5-11, 2005 [poster presented by M. Lodriguito].

129.** M. Włoch, J.R. Gour, K. Kowalski, and P. Piecuch, "The Open-Shell Extension of the Renormalized Equation of Motion Coupled-Cluster Method and its Applications to Many-Electron and Other Many-Fermion Systems," the 45th Sanibel Symposium on Forefront Theory and Computation in Quantum Chemistry, Condensed Matter and Chemical Physics, Nanoscience, Quantum Biochemistry and Biophysics," St. Simons Island, Georgia, U.S.A., March 5-11, 2005 [poster presented by M. Włoch].

130.** K. Kowalski and P. Piecuch, "Extensive Generalization of Renormalized Coupled-Cluster Methods," the 45th Sanibel Symposium on Forefront Theory and Computation in Quantum Chemistry, Condensed Matter and Chemical Physics, Nanoscience, Quantum Biochemistry and Biophysics," St. Simons Island, Georgia, U.S.A., March 5-11, 2005 [invited talk given by K. Kowalski].

131.** D.G. Truhlar, A.W. Jasper, S. Nangia, C. Zhu, P. Piecuch, and M.J. McGuire, "Quantum Photochemistry," John Pople Memorial Symposium, 229th American Chemical Society National Meeting, San Diego, California, U.S.A., March 13-17, 2005 [invited talk given by D.G. Truhlar].

132.** P. Piecuch, M. Włoch, J.R. Gour, and K. Kowalski, "Renormalized and Active-Space Coupled-Cluster Methods: Two Approaches to Electronic Quasi-Degeneracies and Open-Shell Problems," Fifth Congress of the International Society for Theoretical Chemical Physics (ICTCP-V), New Orleans, Louisiana, U.S.A., July 20-26, 2005 [invited plenary talk given by P. Piecuch].

133.** M. Włoch, J.R. Gour, and P. Piecuch, "The Completely Renormalized Coupled-Cluster Approximations Exploiting the Right and Left Eigenstates of the Similarity-Transformed Hamiltonian," Fifth Congress of the International Society for Theoretical Chemical Physics (ICTCP-V), New Orleans, Louisiana, U.S.A., July 20-26, 2005 [poster presented by M. Włoch].

134.** J.R. Gour, M. Włoch, and P. Piecuch, "The Active-Space Equation-of-Motion Coupled-Cluster Method for Electron-Attached and Ionized States," Fifth Congress of the International Society for Theoretical Chemical Physics (ICTCP-V), New Orleans, Louisiana, U.S.A., July 20-26, 2005 [poster presented by J.R. Gour].

135.** S. Coussan, A. Trivella, C. Manca, Y. Ferro, M. Rajzmann, R. Wieczorek, P. Piecuch, K. Kowalski, M. Włoch, S.A. Kucharski, M. Musiał, and P. Roubin, "Acetylacetone Trapped in Inert Matrices: UV and IR Photo-Induced Isomerization and Theoretical Reactional Pathways," The conference "MATRIX-2005, The Physics and Chemistry of Matrix Isolated Species," Funchal, Portugal, July 24-29, 2005 [contributed talk given by S. Coussan].

136.** P. Piecuch, M. Włoch, J.R. Gour, K. Kowalski, A. Kinal, M. Lodriguito, and M.J. McGuire, "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States," The symposium "Theoretical Determination of Energy Landscapes: Methodology and Applications," 230th American Chemical Society National Meeting, Washington, DC, U.S.A., August 28 - September 1, 2005. [invited talk given by P. Piecuch].

137.** P. Piecuch, M. Włoch, and J.R. Gour, "Renormalized and Active-Space Coupled-Cluster Methods: Two Approaches to Quasi-Degeneracies and Open-Shell Problems," Conference on Microscopic Approaches to Many-Body Theory, in honor of Professor Raymond Bishop, The University of Manchester, Manchester, U.K., August 31 - September 3, 2005 [invited talk given by P. Piecuch].

138.** P. Piecuch, J.R. Gour, M. Włoch, and K. Kowalski, "Active-Space Coupled-Cluster Method: An Inexpensive and Highly Accurate Approach to Electronic Quasi-Degeneracies and Open-Shell Problems," Tenth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-X, Carthage, Tunisia, September 1-7, 2005 [invited talk given by P. Piecuch].

139.** P. Piecuch, M. Włoch, and J.R. Gour, "Method of Moments of Coupled-Cluster Equations and Renormalized Coupled-Cluster Approaches to Bond Breaking: A Biorthogonal Size Extensive Formulation," Tenth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-X, Carthage, Tunisia, September 1-7, 2005 [poster presented by P. Piecuch].

140.** P. Piecuch, M. Włoch, J.R. Gour, and A. Kinal, "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [invited plenary lecture given by P. Piecuch].

141.** P. Piecuch and P.-D. Fan, "Intriguing Accuracies of the Exponential Wave Function Expansions Exploiting Finite Two-Body Correlation Operators in Calculations for Many-Electron Systems," 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [poster presented by P. Piecuch].

142.** P. Piecuch, M. Włoch, J.R. Gour, D.J. Dean, T. Papenbrock, and M. Hjorth-Jensen, "Bridging Quantum Chemistry and Nuclear Structure Theory: Coupled-Cluster Calculations for Closed- and Open-Shell Nuclei," 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [poster presented by P. Piecuch].

143.** J.R. Gour, P. Piecuch. and M. Włoch, "Active-Space Equation-of-Motion Coupled-Cluster Methods for Ground and Excited States of Radicals," 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [poster presented by J.R. Gour].

144.** Y. Ohtsuka, P. Piecuch, J.R. Gour, M. Ehara, and H. Nakatsuji, "Extension of the Active-Space Coupled-Cluster Methodology to the Symmetry-Adapted-Cluster Configuration-Interaction Approach," 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [poster presented by J.R. Gour].

145.** M. Włoch, A. Kinal, J.R. Gour, and P. Piecuch, "Single-Reference, Size-Extensive, Non-Iterative Coupled-Cluster Approaches to Bond Breaking and Biradicals," 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [poster presented by M. Włoch].

146.** M. Włoch and P. Piecuch, "Extension of Renormalized Coupled-Cluster Methods Including Triple Excitations to Ground and Excited Electronic States of Open-Shell Molecules," 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [poster presented by M. Włoch].

147.** M.D. Lodriguito, M. Włoch, and P. Piecuch, "Non-iterative Coupled-Cluster Methods Employing Multi-reference Peturbation Theory Wave Functions," 38th Midwest Theoretical Chemistry Conference, Columbus, Ohio June 15-17, 2006 [poster presented by M.D. Lodriguito].

148.** A. Kinal, M.J. McGuire, M. Włoch, and P. Piecuch, "Completely Renormalized Coupled-Cluster and Multi-Reference Configuration Interaction Studies of the Thermal Stereomutations of Cyclopropane," 38th Midwest Theoretical Chemistry Conference, Columbus, Ohio June 15-17, 2006 [contributed talk given by A. Kinal].

149.** P. Piecuch, "Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Bond Breaking and Electronic Excitations in Molecules to Properties of Atomic Nuclei," The Centro Internacional de Matemática Workshop "Mathematics in Chemistry," Lisbon, Portugal, July 19-21, 2006 [invited talk given by P. Piecuch].

150.** P. Piecuch, M. Włoch, J.R. Gour, and A. Kinal, "Advances in Electronic Structure Theory: Single-Reference Coupled-Cluster Methods for Multi-Reference Problems," Sixth Canadian Computational Chemistry Conference (CCCC6), Vancouver, British Columbia, Canada, July 26-30, 2006 [invited plenary talk given by P. Piecuch].

151.** M.D. Lodriguito, M. Włoch, and P. Piecuch, "Non-iterative Coupled-Cluster Methods Employing Multi-reference Peturbation Theory Wave Functions," Sixth Canadian Computational Chemistry Conference (CCCC6), Vancouver, British Columbia, Canada, July 26-30, 2006 [poster presented by M.D. Lodriguito].

152.** P. Piecuch, M. Włoch, A. Kinal, and J.R. Gour, "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," Eleventh European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XI, St. Petersburg, Russia, August 20-25, 2006 [invited talk given by P. Piecuch].

153.** P. Piecuch, M. Włoch, J.R. Gour, D.J. Dean, T. Papenbrock, and M. Hjorth-Jensen, "Bridging Quantum Chemistry and Nuclear Structure Theory: Coupled-Cluster Calculations for Closed- and Open-Shell Nuclei," Eleventh European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XI, St. Petersburg, Russia, August 20-25, 2006 [poster presented by P. Piecuch].

154.** P. Piecuch, J.R. Gour, and M. Włoch, "Active-Space Equation-of-Motion Coupled-Cluster Methods for Ground and Excited States of Radicals," Eleventh European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XI, St. Petersburg, Russia, August 20-25, 2006 [poster presented by P. Piecuch].

155.** C. Sanz, O. Roncero, M.J. McGuire, and P. Piecuch, "Comparative study of the reactive collisions in CaHCl and BeHF systems," MOLEC XVI, European Conference on Dynamics of Molecular Systems, Levico Terme (Trento), Italy, September 11-15, 2006 [poster presented by C. Sanz].

156.** P. Piecuch, "Accurate Quantum Calculations for Many-Body Systems: From Reaction Mechanisms in Organic and Bioinorganic Chemistries to Properties of Atomic Nuclei," Michigan State University High Performance Computing Center 2006 Symposium, East Lansing, Michigan, U.S.A., October 7, 2006 [invited talk].

157.** P. Piecuch, M. Włoch, and J.R. Gour, "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," International Conference "Recent Trends in Many-Body Methods for Electronic Structure and Properties of Atoms and Molecules," Bhubaneswar and Puri, Orissa, India, January 11-13, 2007 [invited talk given by P. Piecuch].

158.** P. Piecuch, J.R. Gour, and M. Włoch, "Active-Space Coupled-Cluster Methods for Bond Breaking, Excited Electronic States, and Open-Shell Systems," International Conference "Practicing Chemistry with Theoretical Tools, on the Occasion of Professor Mark S. Gordon's 65th Birthday," Kihei, Hawaii, U.S.A., January 15-18, 2007 [invited talk given by P. Piecuch].

159.** M.D. Lodriguito and P. Piecuch, "Externally Corrected Coupled-Cluster Methods Employing Method of Moments of Coupled-Cluster Equations and Multi-Reference Perturbation Theory," 233rd American Chemical Society National Meeting, Chicago, Illinois,

March 25-29 (2007) [poster presented by M.D. Lodriguito; Chemical Computing Group Graduate Student Excellence Award].

160.** M. Horoi, J.R. Gour, M. Włoch, M.D. Lodriguito, P. Piecuch, and B.A. Brown, "Coupled-Cluster and Configuration-Interaction Calculations for Heavy Nuclei," Session X16, "Nuclear Theory II," 2007 Americal Physical Society April Meeting, Jacksonville, Florida, U.S.A., April 14-17, 2007 [talk given by M. Horoi].

161.** P. Piecuch, M. Włoch, J.R. Gour, and A. Kinal "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," 39th Midwest Theoretical Chemistry Conference, Indiana University, Bloomington, Indiana, U.S.A., June 28-30, 2007 [invited talk given by P. Piecuch].

162.** J.R. Gour and P. Piecuch, "Active-Space Equation-of-Motion Coupled-Cluster Methods for Ground and Excited States of Radicals," 39th Midwest Theoretical Chemistry Conference, Indiana University, Bloomington, Indiana, U.S.A., June 28-30, 2007 [contributed talk given by J.R. Gour].

163.** Y. Ohtsuka, P. Piecuch, J.R. Gour, M. Ehara, and H. Nakatsuji, "Extension of the Active-Space Coupled-Cluster Methodology to the Symmetry-Adapted-Cluster Configuration-Interaction Approach," 39th Midwest Theoretical Chemistry Conference, Indiana University, Bloomington, Indiana, U.S.A., June 28-30, 2007 [poster presented by J.R. Gour].

164.** J.J. Lutz, P. Piecuch, and A. Kinal, "Extrapolating Potential Energy Surfaces for the Isomerization of Bicyclo[1.1.0]butane to Buta-1,3-diene," 39th Midwest Theoretical Chemistry Conference, Indiana University, Bloomington, Indiana, U.S.A., June 28-30, 2007 [poster presented by J.J. Lutz].

165.** P. Piecuch, "Coupled-Cluster Theory: An Overview of the Basic Formalism and Applications to Molecular and Nuclear Structure Problems," Workshop on Advanced Many-body Methods for Nuclear Structure European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Trento, Italy, July 2-6, 2007 [invited talk given by P. Piecuch].

166.** P. Piecuch, M. Włoch, J.R. Gour, J.J. Lutz, and A. Kinal, "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Applications to Radicals, Biradicals, and Bond Breaking," Twelfth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XII, London, U.K., August 30 - September 5, 2007 [invited talk given by P. Piecuch].

167.** P. Piecuch, M. Włoch, J.R. Gour, J.J. Lutz, and A. Kinal, "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Applications to Radicals, Biradicals, Reaction Pathways, and Photochemistry," "IXth International Conference on Molecular Spectroscopy: From Molecules to Molecular Biological Systems and Molecular Materials, Role of Molecular Interactions and Recognition," Wrocław – Lądek-Zdrój, Poland, September 13-18, 2007 [invited talk given by P. Piecuch].

168.** J.R. Gour, M. Włoch, and P. Piecuch, in collaboration with B.A. Brown, D.J. Dean, M. Hjorth-Jensen, M. Horoi, T. Papenbrock, and R. Roth, "Bridging Quantum Chemistry

and Nuclear Structure Theory: Coupled-Cluster Calculations for Closed- and Open-Shell Nuclei," 2nd Workshop on Nuclei and Mesoscopic Physics, WNMP07, Michigan State University, East Lansing, Michigan, U.S.A., October 20-22, 2007 [poster presented by J.R. Gour].

169.** J.R. Gour, P. Piecuch, and M. Włoch, "Active-Space Equation-of-Motion Coupled-Cluster Methods for Ground and Excited States of Radicals," 2nd Workshop on Nuclei and Mesoscopic Physics, WNMP07, Michigan State University, East Lansing, Michigan, U.S.A., October 20-22, 2007 [poster presented by J.R. Gour].

170.** M. Włoch, J.R. Gour, A. Kinal, and P. Piecuch, "Single-Reference, Size-Extensive, Non-Iterative Coupled-Cluster Approaches to Bond Breaking and Biradicals," 2nd Workshop on Nuclei and Mesoscopic Physics, WNMP07, Michigan State University, East Lansing, Michigan, U.S.A., October 20-22, 2007 [poster presented by J.R. Gour].

171.** J.J. Lutz, P. Piecuch, and A. Kinal, "Extrapolating Potential Energy Surfaces for the Isomerization of Bicyclo[1.1.0]butane to Buta-1,3-diene," 2nd Workshop on Nuclei and Mesoscopic Physics, WNMP07, Michigan State University, East Lansing, Michigan, U.S.A., October 20-22, 2007 [poster presented by J.J. Lutz].

172.** K. Park, P. Piecuch, S.M. Bachrach, T. Nagata, K. Song, and W.L. Hase, "Direct Dynamics Study of the Atomic-Level Mechanism for the Reaction of Cyclopentyne with Ethylene," 63rd Southwest Regional Meeting of the American Chemical Society, Lubbock, Texas, U.S.A., November 3-7, 2007 [poster contribution].

173.** Y. Ge, M.S. Gordon, P. Piecuch, Marta Włoch, and J.R. Gour, "Breaking Bonds of Open-Shell Species with the Restricted Open-Shell Size Extensive Left Eigenstate Completely Renormalized Coupled-Cluster Method," The symposium "Electronic Structure and Reaction Dynamics of Open-shell Species," 235th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., April 6-10, 2008 [contributed talk given by Y. Ge].

174.** P. Piecuch, M. Włoch, and J.R. Gour, "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell Systems," The symposium "Electronic Structure and Reaction Dynamics of Open-shell Species," 235th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., April 6-10, 2008 [invited talk given by P. Piecuch].

175.** J.R. Gour and P. Piecuch, "Active-Space Equation-of-Motion Coupled-Cluster Methods for Ground and Excited States of Radicals and Other Open-Shell Species," The symposium "Electronic Structure and Reaction Dynamics of Open-shell Species," 235th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., April 6-10, 2008 [poster given by J.R. Gour].

176.** J.R. Gour, M. Horoi, P. Piecuch, and B.A. Brown, "Coupled-Cluster and Configuration-Interaction Calculations for Odd-A Heavy Nuclei," The international conference "Nuclear Structure 2008" (NS2008), East Lansing, Michigan, U.S.A., June 3-6, 2008 [poster given by J.R. Gour].

177.** J.J. Lutz, and P. Piecuch, "Extrapolating Potential Energy Surfaces by Sclaing Electron Correlation: Isomerization of Bicyclobutane to Butadiene," 40th Midwest Theoretical Chemistry Conference, University of Michigan, Ann Arbor, Michigan, U.S.A., June 26-28, 2008 [poster presented by J.J. Lutz].

178.** W. Li, J.R. Gour, and P. Piecuch, "Local Correlation Calculations Using Cluster-In-Molecule Standard and Renormalized Coupled-Cluster Methods," 40th Midwest Theoretical Chemistry Conference, University of Michigan, Ann Arbor, Michigan, U.S.A., June 26-28, 2008 [poster presented by W. Li].

179.** J.J. Lutz, and P. Piecuch, "Extrapolating Potential Energy Surfaces by Sclaing Electron Correlation: Isomerization of Bicyclobutane to Butadiene," Thirteenth International Workshop on Quantum Systems in Chemistry and Physics, Michigan State University, East Lansing, Michigan, U.S.A., July 6-12, 2008 [poster presented by J.J. Lutz].

180.** W. Li, J.R. Gour, and P. Piecuch, "Local Correlation Calculations Using Cluster-In-Molecule Standard and Renormalized Coupled-Cluster Methods," Thirteenth International Workshop on Quantum Systems in Chemistry and Physics, Michigan State University, East Lansing, Michigan, U.S.A., July 6-12, 2008 [poster presented by W. Li].

181.** J.R. Gour, P. Piecuch, and M. Ehara "Active-Space Equation-of-Motion Coupled-Cluster Methods for Ground and Excited States of Radicals and Other Open-Shell Species," Thirteenth International Workshop on Quantum Systems in Chemistry and Physics, Michigan State University, East Lansing, Michigan, U.S.A., July 6-12, 2008 [poster presented by J.R. Gour].

182.** J.R. Gour, M. Włoch, and P. Piecuch, "Bridging Quantum Chemistry and Nuclear Structure Theory: Coupled-Cluster Calculations for Closed- and Open-Shell Nuclei," Thirteenth International Workshop on Quantum Systems in Chemistry and Physics, Michigan State University, East Lansing, Michigan, U.S.A., July 6-12, 2008 [poster presented by J.R. Gour].

183.** M. Włoch, P. Piecuch, and J.R. Gour, "Recent Developments and Applications of the Renormalized Coupled-Cluster Methods," Thirteenth International Workshop on Quantum Systems in Chemistry and Physics, Michigan State University, East Lansing, Michigan, U.S.A., July 6-12, 2008 [invited talk given by M. Włoch].

184.** W. Li, J.R. Gour, and P. Piecuch, "Local Correlation Calculations Using Cluster-In-Molecule Standard and Renormalized Coupled-Cluster Methods," The 2008 American Conference on Theoretical Chemistry, Northwestern University, Evanston, Illinois, U.S.A., July 19-24, 2008 [poster presented by W. Li].

185.** P. Piecuch, M. Włoch, J.R. Gour,and W. Li, "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," Sixth Congress of the International Society for Theoretical Chemical Physics (ICTCP-VI), Vancouver, British Columbia, Canada, July 19-24, 2008. [invited plenary talk given by P. Piecuch].

186.** P. Piecuch, "Coupled-Cluster Theory: A Brief Overview of Modern Methods and Applications to Nuclear Structure," the WE-Heraeus-Seminar "Ab-Initio Nuclear Structure -

Where do we stand?", Bad Honnef, Germany, July 28-30, 2008 [invited talk given by P. Piecuch].

187.** J.R. Gour, P. Piecuch, and M. Ehara, "Active-Space Equation-of-Motion Coupled-Cluster Methods for Ground and Excited States of Radicals and Other Open-Shell Systems," Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2008), Sydney, Australia, September 14-19, 2008 [poster presented by J.R. Gour].

188.** J.J. Lutz and P. Piecuch, "Extrapolating Potential Energy Surfaces by Scaling Electron Correlation: Isomerization of Bicyclobutane to Butadiene," Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2008), Sydney, Australia, September 14-19, 2008 [poster presented by J.J. Lutz].

189.** P. Piecuch, M. Włoch, J.R. Gour, and W. Li, "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," 8th World Congress of Theoretically Oriented Chemists (WATOC08), Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2008), Sydney, Australia, September 14-19, 2008 [invited lecture given by P. Piecuch].

190.** W. Li, P. Piecuch, and J.R. Gour, "Local Correlation Calculations Using Cluster-In-Molecule Standard and Renormalized Coupled-Cluster Methods," 8th World Congress of Theoretically Oriented Chemists (WATOC08), Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2008), Sydney, Australia, September 14-19, 2008 [poster presented by P. Piecuch].

191.** P. Piecuch, W. Li, J.R. Gour, and M. Włoch, "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," The International Conference "Theory and Applications of Computational Chemistry 2008 (TACC 2008)," Shanghai, China, September 23-27, 2008 [invited plenary lecture given by P. Piecuch].

192.** J.J. Lutz and P. Piecuch, "Extrapolating Potential Energy Surfaces by Scaling Electron Correlation: Isomerization of Bicyclobutane to Butadiene," Symposium to Honor Professor Peter Wagner in Celebration of his Career and 70th Birthday, Michigan State University, East Lansing, Michigan, U.S.A., October 10-11, 2008 [poster presented by J.J. Lutz].

193.** W. Li, P. Piecuch, and J.R. Gour, "Local Correlation Calculations Using Cluster-In-Molecule Standard and Renormalized Coupled-Cluster Methods," Symposium to Honor Professor Peter Wagner in Celebration of his Career and 70th Birthday, Michigan State University, East Lansing, Michigan, U.S.A., October 10-11, 2008 [poster presented by W. Li].

194.** P. Piecuch, W. Li, and J.R. Gour, "Local Correlation Calculations Using Standard and Renormalized Coupled-Cluster Methods," Focus Session "The Chemical Physics of Biological and Biologically-Inspired Solar Energy Harvesting III," the 2009 American Physical Society March Meeting, Pittsburgh, Pennsylvania, U.S.A., March 16-20, 2009 [associated with the award of Fellowship of APS; contributed talk given by P. Piecuch].

195.** P. Piecuch, W. Li, J.J. Lutz, and J.R. Gour, "Extending Electronic Structure Theory to Complex Molecular Problems: Local Correlation Coupled-Cluster and Correlation Energy Scaling Methodologies," The symposium "Advances in Electronic Structure Theory and First Principles Dynamics," 237th American Chemical Society National Meeting, Salt Lake City, Utah, U.S.A., March 22-26, 2009 [invited talk given by P. Piecuch].

196.** P. Piecuch, "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States," 30th Annual Combustion Research Meeting, Airlie Conference Center, Warrenton, Virginia, U.S.A., May 26-29, 2009 [invited talk given by P. Piecuch].

197.** M. Włoch, P. Piecuch, and J.R. Gour, "Recent Developments and Applications of the Renormalized Coupled-Cluster Methods," 92nd Canadian Chemistry Conference and Exhibition, Hamilton, Ontario, Canada, May 30 - June 3, 2009 [invited talk given by M. Włoch].

198.** P. Piecuch, "Coupled-Cluster Theory: From Quantum Chemistry to Applications in Nuclear Physics," International Workshop "Linking Nuclei, Molecules, and Condensed Matter: Computational Quantum Many-Body Approaches," European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Trento, Italy, July 6-10, 2009 [invited talk given by P. Piecuch].

199.** P. Piecuch, J.R. Gour, W. Li, M. Włoch, and K. Kowalski, "Dealing with Strong Electron Correlations in Quantum Chemistry via Renormalized, Active-Space, and Multi-Reference Coupled-Cluster Methods," The symposium "New Developments in Strongly Correlated Electrons," 238th American Chemical Society National Meeting, Washington, DC, U.S.A., August 16-20, 2009 [invited talk given by P. Piecuch].

200.** P. Piecuch, W. Li, J.J. Lutz, and J.R. Gour, "Extending Electronic Structure Theory to Complex Molecular Problems: Local Correlation Coupled-Cluster and Correlation Energy Scaling Methodologies," Fourteenth International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XIV, San Lorenzo de El Escorial, Madrid, Spain, September 13-19, 2009 [invited talk given by P. Piecuch].

201.** J.R. Gour and P. Piecuch, "Active-Space Electron-Attached and Ionized Equation-of-Motion Coupled-Cluster Methods," Fourteenth International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XIV, San Lorenzo de El Escorial, Madrid, Spain, September 13-19, 2009 [invited talk given by J.R. Gour].

202.** P. Piecuch, J.R. Gour, W. Li, M. Włoch, and K. Kowalski, "Dealing with Strong Electron Correlations in Quantum Chemistry via Renormalized, Active Space, and Multireference Coupled-Cluster Methods," An International Symposium "Recent Advances in Many Electron Theories," Shankarpur, West Bengal, India, January 5-7, 2010 [invited talk given by P. Piecuch].

203.** P. Piecuch and W. Li, "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," the 50th Sanibel Symposium, St. Simons Island, Georgia, U.S.A., February 24-March 2, 2010 [invited talk given by P. Piecuch].

204.** P. Piecuch and W. Li, "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," International conference "Molecular Quantum Mechanics: From Methylene to DNA and Beyond" honoring Professor Henry F. Schaefer's work, University of California at Berkeley, Berkeley, California, U.S.A., May 24-29, 2010 [invited talk given by P. Piecuch].

205.** P. Piecuch and W. Li, "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," 17th Canadian Symposium on Theoretical Chemistry, Edmonton, Alberta, Canada, July 25-30, 2010 [invited talk given by P. Piecuch].

206.** P. Piecuch and W. Li, "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," Fifteenth International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XV, Magdalene College, Cambridge University, Cambridge, U.K., August 31 - September 5, 2010 [invited talk given by P. Piecuch].

207.** P. Piecuch, J. R. Gour, M. Włoch, J. J. Lutz, and W. Li, "Dealing with Chemical Reaction Pathways and Electronic Excitations in Molecular Systems via Renormalized and Active-Space Coupled-Cluster Methods," 18th European Conference on Dynamics of Molecular Systems, MOLEC XVIII, Curia, Portugal, September 5-10, 2010 [invited talk given by P. Piecuch].

208.** P. Piecuch and W. Li, "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," 9th Central European Symposium on Theoretical Chemistry, CESTC 2010, Nový Smokovec, Slovakia, September 12-15, 2010 [invited talk given by P. Piecuch].

209.** P. Piecuch, M. Włoch, J.R. Gour, and W. Li, "Dealing with Chemical Reaction Pathways and Electronic Excitations in Molecular Systems via Renormalized and Active-Space Coupled-Cluster Methods," 8th International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2010), symposium "Methods in Quantum Chemistry" in honor of Jiri Čížek and Josef Paldus, Kos, Greece, October 3-8, 2010 [invited featured lecture, given by P. Piecuch].

210.** P. Piecuch and W. Li, "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," The symposium "Fragment and Local Orbital Methods in Electronic Structure Theory," 241st American Chemical Society National Meeting, Anaheim, California, U.S.A., March 27-31, 2011 [invited talk given by P. Piecuch].

211.** J.A. Hansen, P. Piecuch, J.J. Lutz, and J.R. Gour, "Geometries and Adiabatic Excitation Energies of the Low-Lying States of CNC, C_2N, N_3, and NCO Studied with the Electron-Attached and Ionized Equation-of-Motion Coupled-Cluster Methodologies," Poster session associated with the 2011 Max T. Rogers lectureship, Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., April 6-7, 2011 [poster presented by J.A. Hansen].

212.** J.J. Lutz, G. Fradelos, T.A. Wesołowski, P. Piecuch, and M. Włoch, "Embedding vs Supermolecular Strategies in Evaluating the Hydrogen-Bonding-Induced Shifts of Excitation Energies," Poster session associated with the 2011 Max T. Rogers lectureship, Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., April 6-7, 2011 [poster presented by J.J. Lutz].

213.** W. Li, P. Piecuch, and S. Li, "The Electronic Correlation Method for Large Molecules and its Application in Chemical Reactions," the 11th National Conference of Quantum Chemistry of China, Hefei, China, May 27-30, 2011 [oral contribution presented by W. Li].

214.** P. Piecuch and W. Li, "Local Correlation Coupled-Cluster Methods Exploiting Cluster-In-Molecule Ansatz and their Multi-Level Generalizations," 11th Annual CERMM Symposium, Centre for Research in Molecular Modeling, Concordia University, Montreal, Canada, June 4-5, 2011 [invited keynote lecture given by P. Piecuch].

215.** P. Piecuch, W. Li, J. Shen, J.J. Lutz, and M. Włoch, "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," 94th Canadian Chemistry Conference and Exhibition, General Physical, Theoretical, and Computational Chemistry Session, Montreal, Canada, June 5-9, 2011 [invited lecture given by P. Piecuch].

216.** J.A. Hansen, P. Piecuch, J.J. Lutz, and J.R. Gour, "Geometries and Adiabatic Excitation Energies of the Low-Lying States of CNC, C_2N, N_3, and NCO Studied with the Electron-Attached and Ionized Equation-of-Motion Coupled-Cluster Methodologies," 43rd Midwest Theoretical Chemistry Conference, University of Notre Dame, Indiana, U.S.A., June 9-11, 2011 [poster presented by J.A. Hansen].

217.** J.J. Lutz, G. Fradelos, T.A. Wesołowski, P. Piecuch, and M. Włoch, "Embedding vs Supermolecular Strategies in Evaluating the Hydrogen-Bonding-Induced Shifts of Excitation Energies," 43rd Midwest Theoretical Chemistry Conference, University of Notre Dame, Indiana, U.S.A., June 9-11, 2011 [oral contribution presented by J.J. Lutz].

218.** J. Shen and P. Piecuch, "Merging Active-Space and Renormalized Coupled-Cluster Methods," 43rd Midwest Theoretical Chemistry Conference, University of Notre Dame, Indiana, U.S.A., June 9-11, 2011 [poster presented by J. Shen].

219.** G.R. Magoon, J. Aguilera-Iparraguirre, B. Ruiz-Yi, W.H. Green, O.O. Oluwole, D.K. Lewis, H.-W. Wong, S.E. Albo, J.J. Lutz, and P. Piecuch, "Advanced Development of a Highly Detailed Elementary Combustion Reaction Mechanism for JP-10 (Exotetrahydrodicyclopentadiene)," The 7th International Conference on Chemical Kinetics, Massachusetts Institute of Technology, Cambridge, Massachusetts, U.S.A., July 10-14, 2011 [oral contribution presented by G.R. Magoon].

220.** P. Piecuch and W. Li, "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems and their Multi-Level Generalizations," Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2011), Santiago de Compostela, Spain, July 17-22, 2011 [invited talk given by P. Piecuch].

221.** J.J. Lutz and P. Piecuch, "Performance of Completely Renormalized Equation-Of-Motion Coupled-Cluster Methods on Excited-State Potential Energy Curves for the Dissociation of Water," Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2011), Santiago de Compostela, Spain, July 17-22, 2011 [oral contribution presented by J.J. Lutz].

222.** P. Piecuch, W. Li, J. Shen, J.R. Gour, J.J. Lutz, and M. Włoch, "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," WATOC 2011 Satellite Conference "Strongly Correlated Systems, Cooperativity, and Valence-Bond Theory," A Coruña, Spain, July 23-24, 2011 [invited talk given by P. Piecuch].

223.** J.A. Hansen, P. Piecuch, J.J. Lutz, and J.R. Gour, "Geometries and Adiabatic Excitation Energies of the Low-Lying States of CNC, C_2N, N_3, and NCO Studied with the Electron-Attached and Ionized Equation-of-Motion Coupled-Cluster Methodologies," WATOC 2011 Satellite Conference "Strongly Correlated Systems, Cooperativity, and Valence-Bond Theory," A Coruña, Spain, July 23-24, 2011 [poster presented by J.J. Lutz].

224.** P. Piecuch, W. Li, J. Shen, J.J. Lutz, J.R. Gour, J.A. Hansen, and M. Włoch, "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," The symposium "Reduced Density Matrices in Quantum Chemistry," 242nd American Chemical Society National Meeting, Denver, Colorado, U.S.A., August 28 - September 1, 2011 [invited talk given by P. Piecuch].

225.** P. Piecuch and W. Li, "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems and their Multi-Level Generalizations," The symposium "Quantum Chemistry: Methodology," 242nd American Chemical Society National Meeting, Denver, Colorado, U.S.A., August 28 - September 1, 2011 [talk given by P. Piecuch].

226.** P. Piecuch, G. Fradelos, J.J. Lutz, T.A. Wesołowski, 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," The symposium "Quantum Chemistry: DFT," 242nd American Chemical Society National Meeting, Denver, Colorado, U.S.A., August 28 - September 1, 2011 [talk given by P. Piecuch].

227.** P. Piecuch and W. Li, "Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems and their Multi-Level Generalizations," Seventh Congress of the International Society for Theoretical Chemical Physics (ICTCP-VII), Tokyo, Japan, September 2-8, 2011 [invited talk given by P. Piecuch].

228.** W. Li, P. Piecuch, and S. Li, "Multi-level Extension of the Cluster-In-Molecule Method for the Chemical Reactions of Large Molecules," Seventh Congress of the International Society for Theoretical Chemical Physics (ICTCP-VII), Tokyo, Japan, September 2-8, 2011 [poster presented by W. Li].

229.** G. Fradelos, J.J. Lutz, T.A. Wesołowski, P. Piecuch, and M. Włoch, "Embedding vs Supermolecular Strategies in Evaluating the Hydrogen-Bonding-Induced Shifts of Excitation Energies," Fall 2011 Meeting and General Assembly of the Swiss Chemical Society, Lausanne, Switzerland, September 9, 2011 [poster presented by G. Fradelos].

230.** P. Piecuch, J. Shen, M. Włoch, J.J. Lutz, J.R. Gour, and W. Li, "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," XVI-th International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XVI, Kanazawa, Japan, September 11-17, 2011 [invited talk given by P. Piecuch].

231.** J.A. Hansen, P. Piecuch, J.J. Lutz, and J.R. Gour, "Geometries and Adiabatic Excitation Energies of the Low-Lying States of CNC, C_2N, N_3, and NCO Studied with the Electron-Attached and Ionized Equation-of-Motion Coupled-Cluster Methodologies," Midwestern Symposium on Undergraduate Research in Chemistry, Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., October 7-8, 2011 [poster presented by J.A. Hansen].

232.** N.P. Bauman, P. Piecuch, P.M. Kozłowski, M. Kumar, W. Li, and J.A. Hansen, "Effect of Basis Set on the Cobalt-Methyl Bond Dissociation in Molecular Models of Methyl-Cob(III)alamin Studied with Completely Renormalized Coupled-Cluster Approaches," Midwestern Symposium on Undergraduate Research in Chemistry, Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., October 7-8, 2011 [poster presented by N.P. Bauman].

233.** P. Piecuch, J. Shen, W. Li, J.J. Lutz, M. Włoch, N.P. Bauman, J.A. Hansen, and J.R. Gour, "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," An International Symposium "Recent Advances in Many Electron Theories II, 2011," Puri, Orissa, India, December 1-4, 2011 [invited talk given by P. Piecuch].

234.** P. Piecuch, J. Shen, and W. Li, "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," The Fifth Asian Pacific Conference of Theoretical and Computational Chemistry (APCTCC 2011), Rotorua, New Zealand, December 9-13, 2011 [invited talk given by P. Piecuch].

235.** P. Piecuch, "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States (Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods)," 33rd Annual Combustion Research Meeting, Bolger Center, Potomac, Maryland, U.S.A., May 29 - June 1, 2012 [invited talk given by P. Piecuch].

236.** W. Li, P. Piecuch, Y. Guo, and S. Li, "Cluster-in-Molecule Local Correlation Approach for Chemical Reactions and the Relative Energies of Large Systems," "Low-Scaling and Unconventional Electronic Structure Techniques (LUEST)" Conference, A Satellite Symposium to the 14th International Congress of Quantum Chemistry, Telluride, Colorado, U.S.A., June 18-22, 2012 [poster presented by W. Li].

237.** 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 Bond Breaking, Transition States, and Singlet–Triplet Gaps in Biradical Systems," 14th International Congress of Quantum Chemistry, Boulder, Colorado, U.S.A., June 25-30, 2012 [poster presented by J. Shen].

238.** J.A. Hansen, N.P. Bauman, J. Shen, W.T. Borden, and P. Piecuch, "Low-Lying Electronic States of 1,2,3,4-Cyclobutanetetraone," 14th International Congress of Quantum Chemistry, Boulder, Colorado, U.S.A., June 25-30, 2012 [poster presented by J.A. Hansen].

239.** P.M. Kozlowski, 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," 14th International Congress of Quantum Chemistry, Boulder, Colorado, U.S.A., June 25-30, 2012 [poster presented by P. Piecuch].

240.** N.P. Bauman, P. Piecuch, P.M. Kozlowski, M. Kumar, and J.A. Hansen, "Effect of Basis Set on the Cobalt-Methyl Bond Dissociation in Molecular Models of Methylcobalamin Studied with Completely Renormalized Coupled-Cluster Calculations," 14th International Congress of Quantum Chemistry, Boulder, Colorado, U.S.A., June 25-30, 2012 [poster presented by N.P. Bauman].

241.** P. Piecuch, J. Shen, W. Li, J.R. Gour, J.J. Lutz, M. Włoch, J.A. Hansen, and N.P. Bauman, "Recent Progress in Renormalized and Active-Space Coupled-Cluster Methods," The symposium "Coupled-Cluster Theory and Related Methods," A Satellite Symposium to the 14th International Congress of Quantum Chemistry, Boulder, Colorado, U.S.A., July 1-3, 2012 [invited talk given by P. Piecuch].

242.** P. Piecuch and W. Li, "Multi-level Extensions of the Cluster-in-Molecule Local Correlation Methodology Aimed at Chemical Reaction Pathways Involving Large Molecular Systems," The symposium "Bridging the Gap between *Ab Initio* and Classical Simulations," 244th American Chemical Society National Meeting, Philadelphia, Pennsylvania, U.S.A., August 19-23, 2012 [invited talk given by P. Piecuch].

243.** P. Piecuch and J. Shen, "Combining Active-Space Coupled-Cluster Methods with Moment Energy Corrections via the CC($P;Q$) Methodology, with Benchmark Calculations for Bond Breaking and Biradical Transition States," The symposium "Exploring Potential Energy Surfaces in Quantum Chemistry: A Tribute to H. Bernhard Schlegel," 244th American Chemical Society National Meeting, Philadelphia, Pennsylvania, U.S.A., August 19-23, 2012 [invited talk given by P. Piecuch].

244.** 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 Bond Breaking, Transition States, and Singlet–Triplet Gaps in Biradical Systems," Midwestern Symposium on Undergraduate Research in Chemistry, Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., October 5-6, 2012 [poster presented by J. Shen].

245.** J.A. Hansen, N.P. Bauman, J. Shen, W.T. Borden, and P. Piecuch, "Low-Lying Electronic States of 1,2,3,4-Cyclobutanetetraone," Midwestern Symposium on Undergraduate Research in Chemistry, Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., October 5-6, 2012 [poster presented by J.A. Hansen].

246.** P.M. Kozlowski, 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," Midwestern Symposium on Undergraduate Research in Chemistry, Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., October 5-6, 2012 [poster presented by N.P. Bauman].

247.** P. Piecuch, "Accurate Characterization of Reaction Pathways Relevant to Combustion and Electronic Excitations in Radicals and Biradicals via Renormalized and Active-Space Coupled-Cluster Theories, their Merger, and Open-Shell Extensions," The symposium on Combustion Chemistry, 245th American Chemical Society National Meeting, New Orleans, Lousiana, U.S.A., April 7-11, 2013 [invited talk given by P. Piecuch].

248.** P. Piecuch and J. Shen, "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," The symposium "Quantum Chemistry: Methodology," 245th American Chemical Society National Meeting, New Orleans, Lousiana, U.S.A., April 7-11, 2013 [talk given by P. Piecuch].

249.** P. Piecuch, P.M. Kozłowski, P. Lodowski, M. Jaworska, W. Li, N. Kumar, K. Kornobis, and N.P. Bauman, "The Cobalt-Methyl Dissociation and Electronic Transitions in Methylcobalamin: Insights from the Coupled-cluster, Multireference Perturbation Theory, and Density Functional Theory Calculations," The symposium "Bioinorganic Chemistry: Proteins and Enzymes and Model Systems," 245th American Chemical Society National Meeting, New Orleans, Lousiana, U.S.A., April 7-11, 2013 [talk given by P. Piecuch].

250.** P. Piecuch, W. Li, N.P. Bauman, J.A. Hansen, P.M. Kozłowski, M. Kumar, 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," 45th Midwest Theoretical Chemistry Conference, University of Illinois at Urbana-Champaign, Illinois, U.S.A., May 29-31, 2013 [poster presented by N.P. Bauman].

251.** J.A. Hansen, P. Piecuch, D. Staedter, S. Faure, and V. Blanchet, "Existence of the Doubly Excited State that Mediates the Photoionization of Azulene," 45th Midwest Theoretical Chemistry Conference, University of Illinois at Urbana-Champaign, Illinois, U.S.A., May 29-31, 2013 [contributed talk presented by J.A. Hansen].

252.** P. Piecuch and J. Shen, "Recent Progress in the Active-Space Electron-Attached and Ionized Equation-of-Motion Coupled-Cluster Methodologies," 7th International Conference "Molecular Quantum Mechanics" entitled "Electron Correlation: The Many-Body Problem at the Heart of Chemistry," in honor of Professor Rodney J. Bartlett, Lugano, Switzerland, June 2-7, 2013 [invited talk given by P. Piecuch].

253.** P. Piecuch and J. Shen, "Recent Progress in the Active-Space Electron-Attached and Ionized Equation-of-Motion Coupled-Cluster Methodologies," Eighth Congress of the International Society for Theoretical Chemical Physics (ISTCP-VIII), Budapest, Hungary, August 25-31, 2013 [invited talk given by P. Piecuch].

254.** P. Piecuch, J. Shen, N.P. Bauman, and J.A. Hansen, "Single-Reference Coupled-Cluster Methods for Multi-Reference Molecular Problems," 6th Conference "Current Trends in Theoretical Chemistry" (CTTC VI), Cracow, Poland, September 1-5, 2013 [invited talk given by P. Piecuch].

255.** J.A. Hansen, M. Ehara, and P. Piecuch, "Aerobic Oxidation of Methanol on Au_8^- Cluster by the CR-CC(2,3) and DFT Calculations," The 7th Annual Meeting of Japan Society for Molecular Science, Kyoto, Japan, September 24-27, 2013 [talk given by M. Ehara].

256.** J.A. Hansen, N.P. Bauman, J. Shen, W.T. Borden, and P. Piecuch, "Low-Lying Electronic States of 1,2,3,4-Cyclobutanetetraone," Midwestern Symposium on Undergraduate Research in Chemistry, Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., October 4-5, 2013 [poster presented by J.A. Hansen].

257.** 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," Midwestern Symposium on Undergraduate Research in Chemistry, Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., October 4-5, 2013 [poster presented by N.P. Bauman].

258.** P. Piecuch, J.A. Hansen, V. Blanchet, P.M. Kozłowski, and N. Kumar, "Understanding Photochemistry and Photo-ionization Dynamics with Highly Correlated Electronic Structure Methods: Two Examples that Highlight the Transformative Role of Theory in the Interpretation of Experimental Observations," XVIII-th International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XVIII), Paraty (Rio de Janeiro), Brazil, December 1-7, 2013 [invited talk given by P. Piecuch].

259.** P. Piecuch, J.A. Hansen, V. Blanchet, P.M. Kozłowski, and N. Kumar, "Understanding Photochemistry and Photo-ionization Dynamics with Highly Correlated Electronic Structure Methods: Two Examples that Highlight the Transformative Role of Theory in the Interpretation of Experimental Observations," The symposium "A Little Insight Goes a Long Way," 247th American Chemical Society National Meeting, Dallas, Texas, U.S.A., March 16-20, 2014 [invited talk given by P. Piecuch].

260.** P. Piecuch, J. Shen, and N.P. Bauman, "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(P;Q) Methodology: Connected Triple and Quadruple Excitations," The symposium "Quantum Chemistry: Methodology," 247th American Chemical Society National Meeting, Dallas, Texas, U.S.A., March 16-20, 2014 [talk given by P. Piecuch].

261.** P. Piecuch, J.A. Hansen, M. Ehara, and B.G. Levine, "Utility of New Generations of Coupled-Cluster Methods and Algorithms in Catalytic and Structural Properties of Gold Nanoparticles," The symposium "Quantum Chemistry: Applications," 247th American Chemical Society National Meeting, Dallas, Texas, U.S.A., March 16-20, 2014 [talk given by P. Piecuch].

262.** P. Piecuch, W. Li, N.P. Bauman, J.A. Hansen, P.M. Kozłowski, P. Lodowski, M. Jaworska, M. Kumar, K. Kornobis, and N. Kumar, "The Cobalt-Methyl Dissociation and Electronic Transitions in Methylcobalamin: Insights from Coupled-Cluster, Multireference Perturbation Theory, and Density Functional Theory Calculations," A Symposium on Chemistry and Applications of Advanced Materials in Recognition of Thomas J. Pinnavaia's 47-year MSU Career, Michigan State University, East Lansing, Michigan, U.S.A., May 10, 2014 [poster presented by N.P. Bauman].

263.** J. Shen, N.P. Bauman, and P. Piecuch, "Combining Active-Space Coupled-Cluster Methods with Moment Energy Corrections via the CC(P;Q) Methodology, with Benchmark Calculations for Bond Breaking, Transition States, and Singlet–Triplet Gaps in Biradical Systems," A Symposium on Chemistry and Applications of Advanced Materials in

Recognition of Thomas J. Pinnavaia's 47-year MSU Career, Michigan State University, East Lansing, Michigan, U.S.A., May 10, 2014 [poster presented by N.P. Bauman].

264.** J. Shen and P. Piecuch, "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," A Symposium on Chemistry and Applications of Advanced Materials in Recognition of Thomas J. Pinnavaia's 47-year MSU Career, Michigan State University, East Lansing, Michigan, U.S.A., May 10, 2014 [poster presented by J. Shen and P. Piecuch].

265.** 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 Triple and Quadruple Excitations," The 2014 American Conference on Theoretical Chemistry (ACTC 2014), Telluride, Colorado, U.S.A., July 20-25, 2014 [poster presented by N.P. Bauman].

266.** J. Shen and P. Piecuch, "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," The 2014 American Conference on Theoretical Chemistry (ACTC 2014), Telluride, Colorado, U.S.A., July 20-25, 2014 [poster presented by J. Shen].

267.** P. Piecuch, J. Shen, N.P. Bauman, and J.A. Hansen, "Single-Reference Coupled-Cluster Methods for Multi-Reference Molecular Problems," Nordita program on "Computational Challenges in Nuclear and Many-Body Physics," Stockholm, Sweden, September 15 - October 10, 2014 [invited talk given by P. Piecuch].

268.** P. Piecuch, J. Shen, and N.P. Bauman, "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(P;Q) Methodology," Tenth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2014), Santiago, Chile, October 5-10, 2014 [invited talk given by P. Piecuch].

269.** P. Piecuch and J. Shen, "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," Tenth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2014), Santiago, Chile, October 5-10, 2014 [poster presented by P. Piecuch].

270.** P. Piecuch, J. Shen, and N.P. Bauman, "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(P;Q) Methodology," The Fourteenth Theoretical Chemistry Symposium (TCS 2014), Pune, India, December 18-21, 2014 [invited keynote lecture given by P. Piecuch].

271.** P. Piecuch, J.A. Hansen, and N.P. Bauman, "Understanding Photochemistry and Photoelectron Spectra with Highly Correlated Electronic Structure Methods Based on Coupled-Cluster Theory," The symposium "Modeling Excited States of Complex Systems," 249th American Chemical Society National Meeting, Denver, Colorado, U.S.A., March 22-26, 2015 [invited talk given by P. Piecuch].

272.** P. Piecuch, J.A. Hansen, and M. Ehara, "Aerobic Oxidation of Methanol to Formic Acid on Au_8^-: Benchmark Analysis Based on Completely Renormalized Coupled-Cluster and Density Functional Theory Calculations," The symposium "Computational Chemical Dynamics: Advancing Our Understanding of Chemical Processes in Gas-Phase,

Biomolecular and Condensed-Phase Systems," 249th American Chemical Society National Meeting, Denver, Colorado, U.S.A., March 22-26, 2015 [talk given by P. Piecuch].

273.** P. Piecuch, J. Shen, and N.P. Bauman, "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(P;Q) Methodology: Ground and Excited States," The symposium "Quantum Chemistry: Methodology," 249th American Chemical Society National Meeting, Denver, Colorado, U.S.A., March 22-26, 2015 [talk given by P. Piecuch].

274.** P. Piecuch, "Molecular Systems from the Equation-of-Motion Coupled-Cluster Theory" or "Understanding Electronic Excitation, Multi-Photon Ionization, and Photo-Electron Spectra with the Equation-of-Motion Coupled-Cluster Theory," Workshop of the Espace de Structure Nucléaire Théorique on "Near-Degenerate Systems in Nuclear Structure and Quantum Chemistry from Ab-Initio Many-Body Methods," CEA Saclay, France, March 30 - April 2, 2015 [invited talk given by P. Piecuch].

275.** J. Shen, N.P. Bauman, and P. Piecuch, "Combining Active-Space Coupled-Cluster Methods with Moment Energy Corrections via the CC(P;Q) Methodology, with Benchmark Calculations for Bond Breaking, Transition States, and Singlet–Triplet Gaps in Biradical Systems," Graduate Students Symposium Co-Sponsored by the Dow Chemical Company and the MSU ACS Local Section, Michigan State University, East Lansing, Michigan, U.S.A., April 24, 2015 [poster presented by N.P. Bauman].

276.** P. Piecuch, J. Shen, N.P. Bauman, and J.A. Hansen, "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems," The symposium "Recent Advances in Electronic Structure Theory (RAEST2015)," A Satellite Symposium to the 15th International Congress of Quantum Chemistry, Nanjing, China, June 1-6, 2015 [invited talk given by P. Piecuch].

277.** A.O. Ajala, J.A. Hansen, and P. Piecuch, "Benchmarking the Renormalized Equation-of-Motion Coupled-Cluster Approaches for Vertical Excitation Energies," 47th Midwest Theoretical Chemistry Conference, University of Michigan, Ann Arbor, Michigan, U.S.A., June 26-28, 2015 [poster presented by A.O. Ajala].

278.** N.P. Bauman, J.A. Hansen, P. Piecuch, and M. Ehara, "Coupled-Cluster Interpretation of the Photoelectron Spectra of Ag_3^- and Au_3^-," 47th Midwest Theoretical Chemistry Conference, University of Michigan, Ann Arbor, Michigan, U.S.A., June 26-28, 2015 [contributed talk given by N.P. Bauman].

279.** J.A. Hansen, P. Piecuch, and J. Shen, "Completely Renormalized Coupled-Cluster Calculations for Bond Breaking Using Unrestricted Hartree-Fock References," 47th Midwest Theoretical Chemistry Conference, University of Michigan, Ann Arbor, Michigan, U.S.A., June 26-28, 2015 [contributed talk given by J.A. Hansen].

280.** J. Shen, N.P. Bauman, and P. Piecuch, "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(P;Q) Methodology: Ground and Excited States," 47th Midwest Theoretical Chemistry Conference, University of Michigan, Ann Arbor, Michigan, U.S.A., June 26-28, 2015 [poster presented by J. Shen].

281.** P. Piecuch, J. Shen, and N.P. Bauman, "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Theories for High-Accuracy *Ab Initio* Computations of Chemical Reaction Profiles Involving Biradical Transition States and Electronic Spectra of Radical and Polyradical Species," The symposium "From Diradicals and Polyradicals to Functionalized Materials: Theory Meets Experiment," 250th American Chemical Society National Meeting, Boston, Massachusetts, U.S.A., August 16-20, 2015 [invited talk given by P. Piecuch].

282.** P. Piecuch, J.A. Hansen, N.P. Bauman, and M. Ehara, "Utility of New Generations of Coupled-Cluster Methods and Algorithms in Catalytic, Structural, and Optical Properties of Gold Nanoparticles," The symposium "Interplay between Theory and Experiment in Catalytic Research," the 2015 International Chemical Congress of Pacific Basin Societies (Pacifichem 2015), Honolulu, Hawaii, U.S.A., December 15-20, 2015 [invited talk given by P. Piecuch].

283.** P. Piecuch, N.P. Bauman, and J.A. Hansen, "Coupled-Cluster Interpretation of the Photoelectron Spectra of Ag_3^- and Au_3^-," 26th Austin Symposium on Molecular Structure and Dynamics, Dallas, Texas, U.S.A., March 5-7, 2016 [invited talk given by P. Piecuch].

284.** P. Piecuch, "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States (Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: CC(P;Q) Formalism)," 2nd Computational and Theoretical Chemistry Research PI Meeting, Gaithersburg, Maryland, U.S.A., May 15-18, 2016 [invited talk given by P. Piecuch].

285.** P. Piecuch, J. Shen, N.P. Bauman, and I. Magoulas, "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems," TSRC Workshop "Low-Scaling and Unconventional Electronic Structure Techniques" (LUEST 2016), 3rd edition, Telluride, Colorado, U.S.A., June 1-5, 2016 [invited talk given by P. Piecuch].

286.** P. Piecuch, J. Shen, N.P. Bauman, and I. Magoulas, "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: CC(P;Q) Formalism," Ninth Congress of the International Society for Theoretical Chemical Physics (ISTCP-IX), Grand Forks, North Dakota, U.S.A., July 17-22, 2016 [invited talk given by P. Piecuch].

287.** W. Li, S. Li, J. Ma, and P. Piecuch, "Cluster-in-Molecule and Generalized Energy-Based Fragmentation Coupled Cluster for Large Systems," Ninth Congress of the International Society for Theoretical Chemical Physics (ISTCP-IX), Grand Forks, North Dakota, U.S.A., July 17-22, 2016 [invited talk given by W. Li].

288.** N.P. Bauman, J.A. Hansen, P. Piecuch, and M. Ehara, "Coupled-Cluster Interpretation of the Photoelectron Spectra of Ag_3^- and Au_3^-," Ninth Congress of the International Society for Theoretical Chemical Physics (ISTCP-IX), Grand Forks, North Dakota, U.S.A., July 17-22, 2016 [poster presented by N.P. Bauman].

289.** I. Magoulas, N.P. Bauman, J. Shen, and P. Piecuch, "Application of the CC(P;Q) Hierarchy of Coupled-Cluster Methods to the Challenging Problem of Be_2," Ninth Congress

of the International Society for Theoretical Chemical Physics (ISTCP-IX), Grand Forks, North Dakota, U.S.A., July 17-22, 2016 [poster presented by I. Magoulas].

290.** A.O. Ajala, J. Shen, and P. Piecuch, "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," Ninth Congress of the International Society for Theoretical Chemical Physics (ISTCP-IX), Grand Forks, North Dakota, U.S.A., July 17-22, 2016 [poster presented by A.O. Ajala].

291.** J.E. Deustua, A.O. Ajala, J.A. Hansen, J. Shen, and P. Piecuch, "Benchmarking the Active-Space and Completely Renormalized Equation-of-Motion Coupled-Cluster Approaches for Vertical Excitation Energies," Ninth Congress of the International Society for Theoretical Chemical Physics (ISTCP-IX), Grand Forks, North Dakota, U.S.A., July 17-22, 2016 [poster presented by J.E. Deustua].

292.** P. Piecuch, J. Shen, N.P. Bauman, and I. Magoulas, "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: CC(P;Q) Formalism," The International Conference "Theory and Applications of Computational Chemistry 2016 (TACC 2016)," Seattle, Washington, August 28 - September 2, 2016 [invited talk given by P. Piecuch].

293.** P. Piecuch, N.P. Bauman, and J.A. Hansen, "Understanding Photochemistry and Photoelectron Spectra with Highly Correlated Electronic Structure Methods based on Coupled-Cluster Theory," 7th Conference "Current Trends in Theoretical Chemistry" (CTTC VII), Cracow, Poland, September 4-8, 2016 [invited talk given by P. Piecuch].

294.** P. Piecuch, J. Shen, and A.O. Ajala, "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," EMN Meeting on Computation and Theory (Energy, Materials, and Nanotechnology), workshop "Novel Electron Correlation Methods for Complex Systems," Las Vegas, Nevada, U.S.A., October 10-14, 2016. [invited talk given by P. Piecuch].

295.** P. Piecuch, N.P. Bauman, and J.A. Hansen, "Coupled-Cluster Interpretation of the Photoelectron Spectra of Ag_3^- and Au_3^-," GAMESS*7557*SSEMAG Palindromic Birthday Theory Symposium, on the Occasion of Professor Mark S. Gordon's 75th and Professor Kim K. Baldridge 57th Birthdays," Lihue, Hawaii, U.S.A., January 16-18, 2017 [invited talk given by P. Piecuch].

296.** P. Piecuch, J. Shen, and A.O. Ajala, "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," An International Conference "Recent Advances in Many-Electron Theory (RAMET-2017)," Goa, India, February 9-12, 2017 [invited talk given by P. Piecuch].

297.** P. Piecuch, "The 1966 *Journal of Chemical Physics* Article by Jiří Čížek: What Is in It and Why Is It so Important," the 57th Sanibel Symposium, a special symposium recognizing the 50th Anniversary of Jiří Čížek's 1966 Paper on Coupled-Cluster Theory, St. Simons Island, Georgia, U.S.A., February 19-24, 2017 [invited talk given by P. Piecuch].

298.** A.O. Ajala, J. Shen, and P. Piecuch, "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," 49th Midwest

Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 1-3, 2017 [contributed talk given by A.O. Ajala].

299.** J.E. Deustua, J. Shen, and P. Piecuch, "Benchmarking Completely Renormalized Equation-of-Motion Coupled-Cluster Approaches for Vertical Excitation Energies against Active-Space EOMCCSDt and Full EOMCCSDT Data," 49th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 1-3, 2017 [poster presented by J.E. Deustua].

300.** J. Liu, I. Magoulas, Y. Qi, and P. Piecuch, "Cluster Approach for Predicting the Open Circuit Voltage in Energy Storage Materials Using High-Accuracy Quantum Chemistry Calculations," 49th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 1-3, 2017 [poster presented by J. Liu and I. Magoulas].

301.** J. Shen, N.P. Bauman, I. Magoulas, and P. Piecuch, "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: CC(P;Q) Formalism," 49th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 1-3, 2017 [poster presented by J. Shen].

302.** A.O. Ajala, J. Shen, and P. Piecuch, "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," The 2017 American Conference on Theoretical Chemistry (ACTC 2017), Boston, Massachusetts, U.S.A., July 16-21, 2017 [poster presented by A.O. Ajala].

303.** P. Piecuch, J. Shen, N.P. Bauman, and I. Magoulas, "Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: CC(P;Q) Formalism," The symposium "Electronic Structure of Complex Chemical Systems," 254th American Chemical Society National Meeting, Washington, DC, U.S.A., August 20-24, 2017 [invited talk given by P. Piecuch].

304.** P. Piecuch, J. Shen, and A.O. Ajala, "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," PHYS Awards Symposium, 254th American Chemical Society National Meeting, Washington, DC, U.S.A., August 20-24, 2017 [invited talk given by P. Piecuch].

305.** P. Piecuch, J.E. Deustua, and J. Shen, "Stochastic CC(P;Q) Theory: Converging High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," Eleventh Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2017), Munich, Germany, August 27 - September 1, 2017 [invited talk given by P. Piecuch].

306.** P. Piecuch, J.E. Deustua, and J. Shen, "High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," 15th Central European Symposium on Theoretical Chemistry, CESTC 2017, Wisła, Poland, September 3-6, 2017 [invited talk given by P. Piecuch].

307.** E. Pastorczak, J. Shen, M. Hapka, P. Piecuch, and K. Pernal, "Intriguing van der Waals Interactions Revealed by Electron-Groups Embedding Approach," Wisła, Poland, September 3-6, 2017 [contributed talk given by K. Pernal].

308.** P. Piecuch, J.E. Deustua, and J. Shen, "High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," 27th Austin Symposium on Molecular Structure and Dynamics, Dallas, Texas, U.S.A., March 3-5, 2018 [invited talk given by P. Piecuch].

309.** P. Piecuch, "Introduction to Single-Reference Many-Body Perturbation Theory and its Diagrammatic Representation," Workshop of the Espace de Structure Nucléaire Théorique on "Many-Body Perturbation Theories in Modern Quantum Chemistry and Nuclear Physics," CEA Saclay, France, March 26-30, 2018 [invited introductory lecture given by P. Piecuch].

310.** P. Piecuch, "Perturbative Corrections to Non-perturbative Methods" or "High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," Workshop of the Espace de Structure Nucléaire Théorique on "Many-Body Perturbation Theories in Modern Quantum Chemistry and Nuclear Physics," CEA Saclay, France, March 26-30, 2018 [invited talk given by P. Piecuch].

311.** P. Piecuch, "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," 4th Computational and Theoretical Chemistry Research PI Meeting, Gaithersburg, Maryland, U.S.A., May 21-24, 2018. [invited talk given by P. Piecuch].

312.** P. Piecuch, J.E. Deustua, and J. Shen, "High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," TSRC Workshop "Low-Scaling and Unconventional Electronic Structure Techniques" (LUEST 2018), 4th edition, Telluride, Colorado, U.S.A., June 4-8, 2018 [invited talk given by P. Piecuch].

313.** P. Piecuch, J.E. Deustua, and J. Shen, "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," The joint Annual Workshop on Recent Developments in Electronic Structure Methods (ES18) and Penn Conference in Theoretical Chemistry (PCTC18), Philadelphia, Pennsylvania, U.S.A., June 10-14, 2018 [invited talk given by P. Piecuch].

314.** J.E. Deustua, J. Shen, and P. Piecuch, "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," 50th Midwest Theoretical Chemistry Conference, University of Chicago, Chicago, Illinois, U.S.A., June 21-23, 2018 [poster presented by J.E. Deustua].

315.** I. Magoulas, J. Shen, and P. Piecuch, "Coupled-Cluster Approaches for Strongly Correlated Systems," 50th Midwest Theoretical Chemistry Conference, University of Chicago, Chicago, Illinois, U.S.A., June 21-23, 2018 [poster presented by I. Magoulas].

316.** J. Shen, A.O. Ajala, and P. Piecuch, "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," 50th Midwest Theoretical Chemistry Conference, University of Chicago, Chicago, Illinois, U.S.A., June 21-23, 2018 [poster presented by J. Shen].

317.** S.H. Yuwono, I. Magoulas, N.P. Bauman, J. Shen, and P. Piecuch, "Application of the CC(P;Q) Hierarchy of Coupled-Cluster Methods to the Challenging Beryllium and Magnesium Dimers," 50th Midwest Theoretical Chemistry Conference, University of Chicago, Chicago, Illinois, U.S.A., June 21-23, 2018 [poster presented by S.H. Yuwono].

318.** P. Piecuch, J.E. Deustua, and J. Shen, "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," The symposium "Strong Correlation in Electronic Structure Theory," A Satellite Symposium to the 16th International Congress of Quantum Chemistry, Strasbourg, France, June 24-27, 2018 [invited talk given by P. Piecuch].

319.** P. Piecuch, J.E. Deustua, and J. Shen, "Toward Exact Quantum Chemistry: High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," 28th Canadian Symposium on Theoretical and Computational Chemistry (CSTCC 2018), Windsor, Ontario, Canada, July 15-19, 2018 [invited talk given by P. Piecuch].

320.** P. Piecuch, J.E. Deustua, and J. Shen, and I. Magoulas, "Toward Exact Quantum Chemistry: Accurate Electronic Energies by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," The international conference "Quantum International Frontiers 2018," Changsha, Hunan Province, China, October 17-21, 2018 [invited Frontier Lecture given by P. Piecuch].

321.** P. Piecuch, "Toward Exact Quantum Chemistry by Combining Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Mainz-Kobe Joint Workshop on "Solving the Full Configuration Interaction Problem," RIKEN Center for Computational Science, Kobe, Japan, November 26-27, 2018 [invited talk given by P. Piecuch during teleconference session].

322.** P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, and S.H. Yuwono, "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," TSRC Workshop "New Frontiers in Electron Correlation," 2nd edition, Telluride, Colorado, U.S.A., June 10-14, 2019 [invited talk given by P. Piecuch].

323.** P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, and S.H. Yuwono, "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Tenth Congress of the International Society for Theoretical Chemical Physics (ISTCP-X), symposium entitled "Emergent Electronic Structure Methods," Tromsø, Norway, July 11-17, 2019 [invited talk given by P. Piecuch].

324.** J. Shen, A.O. Ajala, and P. Piecuch, "Efficient Implementation and Applications of the Doubly Electron-Attached and Doubly Ionized Equation-of-Motion Coupled-Cluster Methods," Tenth Congress of the International Society for Theoretical Chemical Physics (ISTCP-X), Tromsø, Norway, July 11-17, 2019 [poster presented by J. Shen].

325.** J.E. Deustua, I. Magoulas, S.H. Yuwono, J. Shen, and P. Piecuch "Accurate Electronic Energies by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster and Equation-of-Motion Coupled-Cluster Computations," Tenth Congress of the International Society for Theoretical Chemical Physics (ISTCP-X), Tromsø, Norway, July 11-17, 2019 [poster presented by J.E. Deustua].

326.** P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, and S.H. Yuwono, "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," 8th Conference "Current Trends in Theoretical

Chemistry" (CTTC VIII), Cracow, Poland, September 1-4, 2019 [invited talk given by P. Piecuch].

327.** P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, and S.H. Yuwono, "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," 20th International Conference on Recent Progress in Many-Body Theories, Toulouse, France, September 9-13, 2019 [invited talk given by P. Piecuch].

328.** P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, S.H. Yuwono, and A. Chakraborty, "Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," The Utah Workshop on Quantum Methods in Molecular and Solid-State Theory, Park City, Utah, U.S.A., September 22-27, 2019 [invited talk given by P. Piecuch].

329.** P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, S.H. Yuwono, and A. Chakraborty, "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Workshop on New Methods for Strongly Correlated Electrons, Qingdao, China, October 9-13, 2019 [invited talk given by P. Piecuch].

330.** P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, S.H. Yuwono, and A. Chakraborty, "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," The international conference "Quantum International Frontiers 2019," Shanghai, China, November 18-22, 2019 [invited Frontier Lecture given by P. Piecuch].

331.** P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, S.H. Yuwono, and A. Chakraborty, "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," the 60th Sanibel Symposium, St. Simons Island, Georgia, U.S.A., February 16-21, 2020 [invited talk given by P. Piecuch].

332.** P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, S.H. Yuwono, A. Chakraborty, and K. Gururangan, "High-Accuracy Electronic Energetics by Stochastic and Deterministic Wave Function Sampling and Coupled-Cluster Computations," TSRC Workshop "Low-Scaling and Unconventional Electronic Structure Techniques" (LUEST 2020), 5th edition, Telluride, Colorado, U.S.A., June 1-5, 2020.
DUE TO COVID-19, REPLACED BY VIRTUAL WORKSHOP, June 1-5 and June 8-9, 2020 [invited talk given by P. Piecuch via Zoom].

333.** P. Piecuch, "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States (Toward Exact Quantum Chemistry)," 2020 Computational and Theoretical Chemistry Virtual Conference Series (July 16, July 30, August 13, 2020), Germantown, Maryland, U.S.A., August 13, 2020 [invited talk given by P. Piecuch via Zoom].

334.** P. Piecuch, "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," The Physical, Theoretical, and Computational Chemistry Virtual Seminar Series, Chemical Institute of Canada, December 1, 2020 [invited talk given by P. Piecuch via Zoom].

335.** P. Piecuch, J. Shen, J.E. Deustua, I. Magoulas, S.H. Yuwono, A. Chakraborty, and K. Gururangan, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," TSRC Workshop "New Frontiers in Electron Correlation," 3rd edition, Telluride, Colorado, U.S.A., June 14-18, 2021 [virtual workshop; invited talk given by P. Piecuch via Zoom].

336.** P. Piecuch, J. Shen, J.E. Deustua, I. Magoulas, S.H. Yuwono, A. Chakraborty, and K. Gururangan, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," The 4th TSRC Workshop "New Developments in Coupled-Cluster Theory," Telluride, Colorado, U.S.A., July 19-23, 2021 [hybrid format; invited talk given by P. Piecuch via Zoom].

337.** J. Lahiri, M. Moemeni, J. Kline, S.H. Yuwono, I. Magoulas, M. Laboe, J. Shen, B. Borhan, P. Piecuch, J.E. Jackson, and G.J. Blanchard, and M. Dantus, "Proton Abstraction Mechanism of the "Super" Photobase FR0-SB," 262nd American Chemical Society National Meeting, Atlanta, Georgia, U.S.A., August 22-26, 2021. [hybrid format; poster presented by J. Lahiri].

338.** P. Piecuch, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations" (with contributions from J.E. Deustua, I. Magoulas, S.H. Yuwono, A. Chakraborty, K. Gururangan, and J. Shen), International Symposium on Correlated Electrons (SymCorrel21), Munich Center for Quantum Science and Technology, Munich, Germany, October 5-7, 2021 [virtual workshop; invited talk given by P. Piecuch via Zoom].

339.** P. Piecuch, S.H. Yuwono, I. Magoulas, and J. Shen, "Computational Studies of FR0-SB, a Novel Organic Compound that Deprotonates Alcohols upon Photoexcitation," International conference in the series "New Horizons in Scientific Software (NHISS 2021)" entitled "Light-Matter Interaction: Theory Meets Experiment," Jeju Island, South Korea, November 22-25, 2021 [hybrid format; invited talk given jointly by P. Piecuch and S.H. Yuwono via Zoom].

340.** P. Piecuch, J.E. Deustua, I. Magoulas, S.H. Yuwono, A. Chakraborty, K. Gururangan, and J. Shen, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," The Seventeenth Theoretical Chemistry Symposium (TCS 2021), Indian Institute of Science Education and Research Kolkata, Mohanpur, Nadia, West Bengal, India, December 11-14, 2021 [virtual symposium; invited plenary lecture given by P. Piecuch].

341.** M. Dantus, J. Lahiri, M. Moemeni, J. Kline, B. Borhan, I. Magoulas, S.H. Yuwono, P. Piecuch, J.E. Jackson, and G.J. Blanchard, "Design Dynamics and Quantum Theory of Reversible Super Photobases," The symposium "Frontiers in Ultrafast Spectroscopy of Photoexcited States," the 2020 International Chemical Congress of Pacific Basin Societies (Pacifichem 2020), Honolulu, Hawaii, U.S.A., December 15-20, 2020 [invited talk given by M. Dantus].
DUE TO COVID-19, RESCHEDULED TO December 16-21, 2021 as hybrid congress.

342.** P. Piecuch, I. Magoulas, K. Gururangan, J.E. Deustua, and J. Shen, "Externally Corrected Coupled-Cluster Methods Using Selected Configuration Interaction and FCIQMC,"

the 61st Sanibel Symposium, invited session on New Directions in CC Theory, St. Simons Island, Georgia, U.S.A., February 13-18, 2022 [in-person invited plenary lecture given by P. Piecuch].

343.** P. Piecuch, J.E. Deustua, I. Magoulas, S.H. Yuwono, A. Chakraborty, K. Gururangan, and J. Shen, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," Chris Cramer 60th Birthday Symposium, 263rd American Chemical Society National Meeting, San Diego, California, U.S.A., March 20-24, 2022 [hybrid symposium; pre-recorded virtual presentation; invited talk given by P. Piecuch].

344.** S. Li, B.C. Jochim, J. Stamm, S.H. Yuwono, P. Piecuch, J.E. Jackson, and M. Dantus, "Strong-Field-Induced Bond Rearrangement in CH_3NCS Ions," 53rd Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics, Orlando, Florida, U.S.A., May 30 - June 3, 2022 [contributed talk given by J. Stamm].

345.** A. Chakraborty, S.H. Yuwono, J.E. Deustua, J. Shen, and P. Piecuch, "Benchmarking the Semi-Stochastic CC(P;Q) Approach for Singlet–Triplet Gaps in Biradicals," 52nd Midwest Theoretical Chemistry Conference, Ohio State University, Columbus, Ohio, U.S.A., June 2-4, 2022 [contributed talk given by A. Chakraborty].

346.** A. Chakraborty, J. Shen, and P. Piecuch, "Quantum-Monte-Carlo-Driven Equation-of-Motion Coupled-Cluster Approaches for Electron Attachment and Ionization: Implementation and Applications," 52nd Midwest Theoretical Chemistry Conference, Ohio State University, Columbus, Ohio, U.S.A., June 2-4, 2022 [poster presented by A. Chakraborty].

347.** S. Basumallick, A. Chakraborty, J. Shen, and P. Piecuch, "Development and Implementation of Semi-Stochastic Double Electron Attachment and Double Ionization Potential Equation-of-Motion Coupled- Cluster Approaches," 52nd Midwest Theoretical Chemistry Conference, Ohio State University, Columbus, Ohio, U.S.A., June 2-4, 2022 [poster presented by S. Basumallick].

348.** P. Piecuch, I. Magoulas, K. Gururangan, J.E. Deustua, and J. Shen, "Recent Advances in Externally Corrected Coupled-Cluster Methods," 10th International Conference "Molecular Quantum Mechanics" entitled "Molecular Quantum Mechanics: Innovation, Impact, and Insight," in honor of Professors Gustavo Scuseria and Martin Head-Gordon, Blacksburg, Virginia, U.S.A., June 26 - July 1, 2022 [invited plenary lecture given by P. Piecuch].

349.** P. Piecuch, J.E. Deustua, I. Magoulas, S.H. Yuwono, A. Chakraborty, K. Gururangan, and J. Shen, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," Twelfth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2020), Vancouver, British Columbia, Canada, August 16-21, 2020 [invited talk given by P. Piecuch].
DUE TO COVID-19, RESCHEDULED TO July 3-8, 2022.

350.** P. Piecuch, J.E. Deustua, I. Magoulas, S.H. Yuwono, A. Chakraborty, K. Gururangan, and J. Shen, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," The 2020 American Conference on

Theoretical Chemistry (ACTC 2020), Palisades Tahoe (formerly Squaw Valley), California, U.S.A., July 26-30, 2020 [invited talk given by P. Piecuch].
DUE TO COVID-19, RESCHEDULED TO July 24-28, 2022; renamed ACTC 2022.

351.** A. Chakraborty, S.H. Yuwono, J.E. Deustua, J. Shen, and P. Piecuch, "Application of the Semi-Stochastic CC(P;Q) Approach to Singlet–Triplet Gaps in Biradical Systems," The 2020 American Conference on Theoretical Chemistry (ACTC 2020), Palisades Tahoe (formerly Squaw Valley), California, U.S.A., July 26-30, 2020 [poster presented by A. Chakraborty].
DUE TO COVID-19, RESCHEDULED TO July 24-28, 2022; renamed ACTC 2022.

352.** P. Piecuch, I. Magoulas, K. Gururangan, J.E. Deustua, and J. Shen, "Recent Advances in Externally Corrected Coupled-Cluster Methods," The symposium "Quantum Chemistry: Current and Future Frontiers," 264th American Chemical Society National Meeting, Chicago, Illinois, U.S.A., August 21-25, 2022 [in-person and virtual meeting; in-person invited talk given by P. Piecuch].

353.** P. Piecuch, I. Magoulas, K. Gururangan, J.E. Deustua, and J. Shen, "Recent Advances in Externally Corrected Coupled-Cluster Methods," OPERA-2020 (Operators, Perturbations, Electrons, Relativity, and Multi-Scale Applications), an international symposium on theoretical chemistry in honour of Prof. Jürgen Gauss on the occasion of his 60th birthday, Ingelheim am Rhein, Germany, September 1-3, 2021 [invited talk given by P. Piecuch].
DUE TO COVID-19, RESCHEDULED TO August 31 - September 2, 2022.

354.** P. Piecuch, J.E. Deustua, I. Magoulas, S.H. Yuwono, A. Chakraborty, and J. Shen, "Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations," Modeling and Design of Molecular Materials 2020 (MDMM 2020) Conference, Gdańsk, Poland, September 21-24, 2020 [invited talk given by P. Piecuch].
DUE TO COVID-19, RESCHEDULED TO September 19-22, 2022; renamed MDMM 2022.

355.** P. Piecuch, J.E. Deustua, I. Magoulas, S.H. Yuwono, A. Chakraborty, K. Gururangan, and Jun Shen, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," International conference in the series "New Horizons in Scientific Software (NHISS 2022)" entitled "The New Collaborative Platform Goes Life," Jeju Island, South Korea, December 12-15, 2022 [hybrid format; invited talk given by P. Piecuch via Zoom].

356.** P. Piecuch, S.H. Yuwono, I. Magoulas, and J. Shen, "Computational Studies of FR0-SB, a Novel Organic Compound that Deprotonates Alcohols upon Photoexcitation," 28th Austin Symposium on Molecular Structure and Dynamics, Dallas, Texas, U.S.A., February 17-20, 2023 [invited talk given by P. Piecuch].

357.** A. Chakraborty, S.H. Yuwono, J.E. Deustua, J. Shen, and P. Piecuch, "Exploring Electronic Excitations in Molecules and Singlet–Triplet Gaps in Biradicals: A Semi-Stochastic CC(P;Q) Study," 53rd Midwest Theoretical Chemistry Conference, Purdue

University, West Lafayette, Indiana, U.S.A., June 1-3, 2023 [poster presented by A. Chakraborty].

358.** S.S. Priyadarsini, K. Gururangan, J. Shen, and P. Piecuch, "The Singlet–Triplet Gap of Cyclobutadiene: The CIPSI-Driven CC(P;Q) Study," 53rd Midwest Theoretical Chemistry Conference, Purdue University, West Lafayette, Indiana, U.S.A., June 1-3, 2023 [poster presented by S.S. Priyadarsini].

359.** J. Stamm, S. Kwon, C. Wicka, S. Priyadarsini, A. Chakraborty, J. Shen, P. Piecuch, and M. Dantus, "H_3^+ Formation from Methyl Halogens and Pseudohalogens," 54th Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics, Spokane, Washington, U.S.A., June 5-9, 2023 [contributed talk given by J. Stamm].

360.** A. Chakraborty, S.H. Yuwono, J.E. Deustua, J. Shen, and P. Piecuch, "Application of the Semi-Stochastic CC(P;Q) Approach for Electronic Excitations in Molecules and Singlet–Triplet Gaps in Biradicals," The symposium "Computational Chemistry From Electrons to Macromolecules," the 2023 Central Regional Meeting of the American Chemical Society (CERM 2023), Dearborn, Michigan, U.S.A., June 20-23, 2023 [invited talk given by A. Chakraborty].

361.** S.S. Priyadarsini, K. Gururangan, J. Shen, and P. Piecuch, "Potential Energy Curves and the Singlet–Triplet Gap of Cyclobutadiene: CIPSI-driven CC(P;Q) Study," The symposium "Computational Chemistry From Electrons to Macromolecules," the 2023 Central Regional Meeting of the American Chemical Society (CERM 2023), Dearborn, Michigan, U.S.A., June 20-23, 2023 [invited talk given by S.S. Priyadarsini].

362.** P. Piecuch, I. Magoulas, K. Gururangan, J.E. Deustua, T. Deng, and J. Shen, "Externally Corrected Coupled-Cluster Methods: Review and Recent Progress," The symposium "Strong Correlation in Molecules," A Satellite Symposium to the 17th International Congress of Quantum Chemistry, Znojmo, Czech Republic [special invited lecture given by P. Piecuch during the session dedicated to the memory of Josef Paldus].
DUE TO COVID-19, RESCHEDULED TO June 20-23, 2023.

363.** P. Piecuch, J.E. Deustua, K. Gururangan, A. Chakraborty, S.H. Yuwono, S. Priyadarsini, and J. Shen, "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches," 17th International Congress of Quantum Chemistry, Bratislava, Slovakia, June 21-26, 2021 [invited plenary lecture given by P. Piecuch].
DUE TO COVID-19, RESCHEDULED TO June 26 - July 1, 2023.

364.** A. Chakraborty, S.H. Yuwono, J.E. Deustua, J. Shen, and P. Piecuch, "Exploring Electronic Excitations in Molecules and Singlet–Triplet Gaps in Biradicals: A Semi-Stochastic CC(P;Q) Study," The 2023 Telluride School on Theoretical Chemistry, Telluride, Colorado, July 11-16, 2023 [poster presented by A. Chakraborty].

365.** J. Stamm, S. Kwon, C. Wicka, A. Chakraborty, S. Priyadarsini, J. Shen, P. Piecuch, and M. Dantus, "H_3^+ Formation from CH_3X for X = Halogens and Pseudo Halogens," The 15th Femtochemistry Conference (FEMTO 15), Berlin, Germany, July 30 - August 4, 2023 [contributed talk presented by M. Dantus].

366.** P. Piecuch, S.H. Yuwono, I. Magoulas, and J. Shen, "Computational Studies of FR0-SB, a Novel Organic Compound that Deprotonates Alcohols upon Photoexcitation," The 41st Midwest Undergraduate Computational Chemistry Consortium (MU3C) Conference, Michigan State University, East Lansing, Michigan, U.S.A., August 1-2, 2023 [invited talk given by P. Piecuch].

367.** A. Chakraborty, S.H. Yuwono, J.E. Deustua, J. Shen, and P. Piecuch, "Exploring Electronic Excitations in Molecules and Singlet–Triplet Gaps in Biradicals: A Semi-Stochastic CC(P;Q) Study," The 41st Midwest Undergraduate Computational Chemistry Consortium (MU3C) Conference, Michigan State University, East Lansing, Michigan, U.S.A., August 1-2, 2023 [poster presented by A. Chakraborty].

368.** S.S. Priyadarsini, K. Gururangan, J. Shen, and P. Piecuch, "The Singlet–Triplet Gap of Cyclobutadiene: The CIPSI-Driven CC(P;Q) Study," The 41st Midwest Undergraduate Computational Chemistry Consortium (MU3C) Conference, Michigan State University, East Lansing, Michigan, U.S.A., August 1-2, 2023 [poster presented by S.S. Priyadarsini].

369.** S.H. Yuwono, I. Magoulas, N.P. Bauman, J. Shen, and P. Piecuch, "Application of the CC(P;Q) Hierarchy of Coupled-Cluster Methods to the Challenging Problems of Be_2 and Mg_2," The 41st Midwest Undergraduate Computational Chemistry Consortium (MU3C) Conference, Michigan State University, East Lansing, Michigan, U.S.A., August 1-2, 2023 [poster presented by P. Piecuch].

370.** I. Magoulas, J. Shen, and P. Piecuch, "Coupled-Cluster Approaches for Strongly Correlated Systems," The 41st Midwest Undergraduate Computational Chemistry Consortium (MU3C) Conference, Michigan State University, East Lansing, Michigan, U.S.A., August 1-2, 2023 [poster presented by P. Piecuch].

371.** P. Piecuch, J.E. Deustua, K. Gururangan, A. Chakraborty, S.H. Yuwono, S. Priyadarsini, and Jun Shen, "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches," The 5th Conference on Theory and Applications of Computational Chemistry (TACC 2020), Sapporo, Japan, September 7-12, 2020 [invited talk given by P. Piecuch].
DUE TO COVID-19, RESCHEDULED TO September 4-9, 2023; renamed TACC 2023.

372.** P. Piecuch, J.E. Deustua, K. Gururangan, A. Chakraborty, S.H. Yuwono, S. Priyadarsini, and Jun Shen, "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches," 26th International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XXVI), Jaipur, Rajasthan, India, October 14-20, 2023 [hybrid format; invited talk given by P. Piecuch via Zoom].

373.** P. Piecuch, I. Magoulas, K. Gururangan, J.E. Deustua, T. Deng, and J. Shen, "Recent Progress in Externally Corrected Coupled-Cluster Methods: Following the Footsteps of a Legend (Lecture in Memory of Professor Josef Paldus)," The 37th Symposium on Chemical Physics at the University of Waterloo, Waterloo, Ontario, Canada, November 3-5, 2023 [special invited lecture in memory of Josef Paldus given by P. Piecuch].

374.** P. Piecuch, I. Magoulas, J.E. Deustua, T. Deng, and J. Shen, "Addressing Strong Correlations Using Approximate Coupled-Pair Ideas: Following the Footsteps of a Legend (Lecture in Memory of Professor Josef Paldus)," the 63rd Sanibel Symposium, invited session on Coupled-Cluster Theory, St. Augustine Beach, Florida, U.S.A., February 25 - March 1, 2024 [invited plenary lecture given by P. Piecuch].

375.** K. Gururangan and P. Piecuch, "Converging High-Level Coupled-Cluster Energetics via Adaptive Selection of Excitation Manifolds Driven by Moment Expansions," the 63rd Sanibel Symposium, St. Augustine Beach, Florida, U.S.A., February 25 - March 1, 2024 [poster presented by K. Gururangan].

376.** K. Gururangan and P. Piecuch, "Converging High-Level Coupled-Cluster Energetics via Adaptive Selection of Excitation Manifolds Driven by Moment Expansions," 54th Midwest Theoretical Chemistry Conference, University of Wisconsin–Madison, Madison, Wisconsin, U.S.A., May 30 - June 1, 2024 [contributed talk given by K. Gururangan].

377.** T. Deng, J. Shen, and P. Piecuch, "Benchmarking Approximate Coupled-Pair, Completely Renormalized, Active-Space, and CC(P;Q) Coupled-Cluster Methods against DMRG for Singlet–Triplet Gaps in Polyacenes," 54th Midwest Theoretical Chemistry Conference, University of Wisconsin–Madison, Madison, Wisconsin, U.S.A., May 30 - June 1, 2024 [poster presented by T. Deng].

378.** S.S. Priyadarsini, J. Stamm, S. Sandhu, A. Chakraborty, J. Shen, S. Kwon, J. Sandhu, C. Wicka, A. Mehmood, B.G. Levine, P. Piecuch, and M. Dantus, "H_3^+ Formation from Methyl Halogens and Pseudohalogens: Experiment, Theory, and Governing Factors," 54th Midwest Theoretical Chemistry Conference, University of Wisconsin–Madison, Madison, Wisconsin, U.S.A., May 30 - June 1, 2024 [poster presented by S.S. Priyadarsini].

379.** J. Shen, I. Magoulas, and P. Piecuch, "Recent Automated Implementations of Novel Coupled-Cluster and Equation-of-Motion Coupled-Cluster Approaches in GAMESS," 54th Midwest Theoretical Chemistry Conference, University of Wisconsin–Madison, Madison, Wisconsin, U.S.A., May 30 - June 1, 2024 [poster presented by J. Shen].

380.** P. Piecuch, "Remembering Professor Josef Paldus: Pioneer of Modern Electronic Structure Theory and Caring Mentor, Educator, and Friend," Symposium "Advances in Electronic Structure Theory: A Symposium in Honour of Joe Paldus," the 107th Canadian Chemistry Conference and Exhibition (CSC 2024), Winnipeg, Manitoba, Canada, June 2-6, 2024 [invited lecture given by P. Piecuch].

381.** S.S. Priyadarsini, K. Gururangan, J. Shen, and P. Piecuch, "The Singlet–Triplet Gap of Cyclobutadiene: The CIPSI-Driven CC(P;Q) Study," The 2024 American Conference on Theoretical Chemistry (ACTC 2024), University of North Carolina at Chapel Hill, Chapel Hill, North Carolina, U.S.A., June 17-20, 2024 [poster presented by S.S. Priyadarsini].

382.** J. Stamm, S. Sandhu, A. Chakraborty, S. Priyadarsini, J. Shen, S. Kwon, J. Sandhu, C. Wicka, A. Mehmood, B. Levine, P. Piecuch, and M. Dantus, "H^{3+} Formation from Methyl Halogens andPseudohalogens:a Experiments, Theory, and Predictions," The 23rd International Conference on Ultrafast Phenomena, Barcelona, Spain, July 14-19, 2024 [poster presented by M. Dantus].

383.** P. Piecuch, K. Gururangan, J.E. Deustua, A. Chakraborty, S.H. Yuwono, S.S. Priyadarsini, and J. Shen, "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches," 30th Canadian Symposium on Theoretical and Computational Chemistry (CSTCC 2024), Halifax, Nova Scotia, Canada, July 21-25, 2024 [invited lecture given by P. Piecuch].

384.** P. Piecuch, K. Gururangan, J.E. Deustua, A. Chakraborty, S.H. Yuwono, S.S. Priyadarsini, and J. Shen, "Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches," The 5th TSRC Workshop "New Developments in Coupled-Cluster Theory," Telluride, Colorado, U.S.A., July 29 - August 2, 2024 [invited lecture given by P. Piecuch].

385.** S.S. Priyadarsini, K. Gururangan, J. Shen, and P. Piecuch, "The Singlet–Triplet Gap of Cyclobutadiene: The CIPSI-Driven CC(P;Q) Study," MQC Entanglement 2024, the 3rd annual meeting of the Midwest Quantum Collaboratory (MQC), Michigan State University, East Lansing, Michigan, U.S.A., August 5-6, 2024 [poster presented by S.S. Priyadarsini].

386.** T. Deng, J. Shen, and P. Piecuch, "Benchmarking Approximate Coupled-Pair, Completely Renormalized, Active-Space, and CC(P;Q) Coupled-Cluster Methods against DMRG for Singlet–Triplet Gaps in Polyacenes," MQC Entanglement 2024, the 3rd annual meeting of the Midwest Quantum Collaboratory (MQC), Michigan State University, East Lansing, Michigan, U.S.A., August 5-6, 2024 [poster presented by T. Deng].

387.** P. Piecuch, K. Gururangan, J.E. Deustua, A. Chakraborty, S.H. Yuwono, S.S. Priyadarsini, and J. Shen, "Converging High-Level Coupled-Cluster Energetics with Semi-Stochastic, CIPSI-Driven, and Adaptive CC(P;Q) Methods," 9th Conference "Current Trends in Theoretical Chemistry" (CTTC IX), Cracow, Poland, September 1-5, 2024 [invited lecture given by P. Piecuch].

388.** P. Piecuch, K. Gururangan, J.E. Deustua, A. Chakraborty, S.H. Yuwono, S.S. Priyadarsini, and J. Shen, "Converging High-Level Coupled-Cluster Energetics with Semi-Stochastic, CIPSI-Driven, and Adaptive CC(P;Q) Methods," Eleventh Congress of the International Society for Theoretical Chemical Physics (ISTCP-XI), symposium on Wave Function Theory for Electronic Structure, Qingdao, China, October 13-18, 2024 [invited lecture to be given by P. Piecuch].

389.** P. Piecuch, "Remembering Professor Josef Paldus: Pioneer of Modern Electronic Structure Theory and Caring Mentor, Educator, and Friend," Eleventh Congress of the International Society for Theoretical Chemical Physics (ISTCP-XI), Auqing Tang, Joe Paldus, and Bogumił Jeziorski Memorial Symposium and session on Chemical Insights, Qingdao, China, October 13-18, 2024 [invited lecture to be given by P. Piecuch].

390.** TBD, The symposium "Methods and Applications on Simulating Excited States: Molecular Dynamics, Spectroscopy, and Catalysis," 269th American Chemical Society National Meeting, San Diego, California, U.S.A., March 23-27, 2025 [invited lecture to be given by P. Piecuch].

391.** TBD, 11th Molecular Quantum Mechanics Conference (MQM 2025), in honor of Professors Hiroshi Nakatsuji and Kimihiko Hirao and in memory of Professors Keiji Morokuma

and Shigeki Kato, Kyoto, Japan, May 23-28, 2025 [invited lecture to be given by P. Piecuch].