Curriculum Vitae

Dr. Jun Shen, Senior Research Associate
Department of Chemistry, Michigan State University
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Education

Ph. D., 2008, Physical Chemistry, Nanjing University, P. R. China

Research Experience

Senior Research Associate, Department of Chemistry, Michigan State University, 2016- present
Research Associate, Department of Chemistry, Michigan State University, 2014-2016
Assistant Professor (fixed-term), Department of Chemistry, Michigan State University, 2013-2014
Postdoctoral Research Associate, Department of Chemistry, Michigan State University, 2010-2013
Postdoctoral Research Associate, Physics School, Nanjing University, P. R. China, 2008-2010

Research Interests

Theoretical and computational chemistry, in particular: electron correlation structure methods; automatically deriving and coding coupled-cluster theory for both ground state and excited states; new algorithms and computer codes for quantum chemistry; accurate *ab initio* calculations of molecular potential energy surfaces and excited states; linear scaling algorithms for electronic structure calculations.

Awards and Honors

The outstanding Postdoctoral Research Associate of Nanjing University, 2011

The Chinese outstanding graduate student award (twice), 2006, 2008

Graduate and Postdoctoral Advisors

Professor Shuhua Li, School of Chemistry and Chemical Engineering, Nanjing University, China, Ph. D. and postdoctoral advisor

Professor Piotr Piecuch, Department of Chemistry, Michigan State University, postdoctoral advisor

List of Publications:

Book Chapters:

1) J. Shen, T. Fang, and S. Li, "Performance of block correlated coupled cluster method with the CASSCF reference function for carbon–carbon bond breaking in hydrocarbons," 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, S. Wilson, P. J. Grout, J. Maruani, G. Delgado-Barrio, and S. Wilson (Springer, Dordrecht, 2009), pp. 241-255.

2) T. Fang, J. Shen, and S. Li. "Block correlated coupled cluster theory with a complete active-space self-consistent-field reference function: The general formalism and applications," in *Recent Progress in Coupled Cluster Methods: Theory and Applications*, Vol. 11, *Challenges and Advances in Computational Chemistry and Physics*, edited by P. Carsky, J. Paldus, and J. Pittner (Springer, Dordrecht, 2010), pp. 145-174.

Articles:

3) S. Li, J. Shen, W. Li, and Y. Jiang, "An efficient implementation of the "cluster-in-molecule" approach for local electron correlation calculations". *J. Chem. Phys.* **125**, 074109 (2006).

4) J. Shen, T. Fang, W. Hua, and S. Li. "Spectroscopic Constants of Single-Bond Diatomic Molecules and Singlet-Triplet Gaps of Diradicals by the Block-Correlated Coupled Cluster Theory," *J. Phys. Chem. A.* **112**, 4703-4709 (2008).

5) T. Fang, J. Shen, and S. Li, "Block correlated coupled cluster method with a complete-active-space self-consistent-field reference function: The formula for general active spaces and its applications for multibond breaking systems," *J. Chem. Phys.* **128**, 224107 (2008).

6) J. Shen, T. Fang, and S. Li, "Singlet-triplet gaps in substituted carbenes predicted from block-correlated coupled cluster method," *Sci. China Ser. B* **51**, 1197-1202 (2008).

7) J. Shen, T. Fang, S. Li and Y. Jiang, "Performance of Block Correlated Coupled Cluster Method with the CASSCF Reference Function for the Prediction of

Activation Barriers, Spectroscopic Constants in Diatomic Molecules, and Singlet-Triplet Gaps in Diradicals," *J. Phys. Chem. A.* **112**, 12518-12525 (2008).

8) J. Shen, T. Fang, S. Li and Y. Jiang, "Potential Energy Surface for Single-bond Breaking in Alkanes: Study from by Block Correlated Coupled Cluster Method with the CASSCF Reference Function," *Chem. J. Chinese Univ.* **29**, 2341-2344 (2008).

9) T. Fang, J. Shen, and S. Li, "Block correlated coupled cluster method with a complete-active-space self-consistent-field reference function: The implementation for low-lying excited states," *J. Chem. Phys.* **129**, 234106 (2008).

10) J. Shen and S. Li, "Block correlated coupled cluster method with the complete-active-space self-consistent-field reference function: Applications for low-lying electronic excited states," *J. Chem. Phys.* **131**, 174101 (2009).

11) J. Shen and S. Li, "Comparison of some multireference electronic structure methods in illustrative applications," *Sci. China Ser. B* **53**, 289-296 (2010).

12) J. Shen, E. Xu, Z. Kou, and S. Li, "A coupled cluster approach with a hybrid treatment of connected triple excitations for bond-breaking potential energy surfaces," *J. Chem. Phys.* **132**, 114115 (2010).

13) E. Xu, J. Shen, Z. Kou, and S. Li, "Coupled cluster with singles, doubles, and partial higher-order excitations based on the corresponding orbitals: The formulation and test applications for bond breaking processes," *J. Chem. Phys.* **132**, 134110 (2010).

14) J. Shen, Z. Kou, E. Xu, and S. Li, "A coupled cluster approach with a hybrid treatment of connected triple excitations: Implementation and applications for open-shell systems," *J. Chem. Phys.* **133,** 234106 (2010).

15) J. Shen, E. Xu, Z. Kou, and S. Li, "New coupled cluster approaches based on the unrestricted Hartree-Fock reference for treating molecules with multireference character," *Phys. Chem. Chem. Phys. (perspective)* **13**, 8795-8804 (2011).

16) J. Shen, Z. Kou, E. Xu, and S. Li, "The coupled cluster approach with a hybrid treatment of connected triple excitations based on the restricted Hartree-Fock reference," *J. Chem. Phys.* **134,** 044134 (2011).

17) J. Shen, Z. Kou, E. Xu, and S. Li, "The coupled cluster singles, doubles, and a hybrid treatment of connected triples based on the split virtual orbitals," *J. Chem. Phys.* **136,** 044101 (2012).

18) Z. Kou, J. Shen, E. Xu, and S. Li, "Hybrid coupled cluster methods: combining active space coupled cluster methods with coupled cluster singles, doubles, and perturbative triples," *J. Chem. Phys.* **136,** 194105 (2012).

19) Z. Kou, J. Shen, E. Xu, and S. Li, "The coupled cluster approach with a hybrid treatment of connected triple excitations: Spectroscopic constants in open-shell

diatomic molecules, and bond-breaking or twisting potential energy surfaces," *Chem. Phys.* **401,** 113-118 (2012).

20) 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).

21) 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 (2012).

22) 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).

23) Z. Kou, J. Shen, E. Xu, and S. Li, "Hybrid Coupled Cluster Methods Based on the Split Virtual Orbitals: Barrier Heights of Reactions and Spectroscopic Constants of Open-Shell Diatomic Molecules," *J. Phys. Chem. A* **117,** 626-632 (2013).

24) 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 (2013).

25) J. Shen and P. Piecuch, "Doubly Electron-Attached and Doubly Ionized 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).

26) 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).

27) 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).

28) J. Zou, J. Shen, E. Xu, T. Fang, and S. Li, "Multireference Perturbation Theory and Multireference Coupled Cluster Theory Based on the 'Block-Correlation' Framework," *Acta Phys. -Chim. Sin.* **33,** 0001-0009 (2017).

29) A.O. Ajala, J. Shen, and P. Piecuch, "Economical Doubly Electron-Attached Equation-of-Motion Coupled-Cluster Methods with an Active-Space Treatment of 3-particle-1-hole and 4-particle-2-hole Excitations," *J. Phys. Chem. A*, **121**, 3469-3485 (2017).

30) 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).

31) 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).

32) S.J. Stoneburner, J. Shen, A.O. Ajala, P. Piecuch, D. 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 (2017).

33) 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 (2017).

34) I. Magoulas, N.P. Bauman, J. Shen, and P. Piecuch, "Application of the CC(*P*;*Q*) Hierarchy of Coupled-Cluster Methods to Beryllium Dimer," *J. Phys. Chem. A*, **122**, 1350-1368 (2018).

35) 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 (2018).

36) S.H. Yuwono, I. Magoulas, J. Shen, and P. Piecuch, "Application of the CC(*P*;*Q*) Hierarchy of Coupled-Cluster Methods to the Mg_2 Dimer," *Mol. Phys*, **117**, 1486 (2019).

37) 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 (2019).

38) 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. W loch, P. Xu, F. Zahariev, and M.S. Gordon, "Recent Developments in the General Atomic and Molecular Electronic Structure System," *J. Chem. Phys.* **152**, 154102 (2020) [Special Topic Collection "Electronic Structure Software"; invited contribution].

39) 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**, (2020) [Special

Issue in Honour of Professor Jürgen Gauss; invited contribution, in response to an invitation issued to P. Piecuch].

40) J. Lahiri, M. Moemeni, J. Kline, I. Magoulas, S.H. Yuwono, M. Laboe, J. Shen, B. Borhan, P. Piecuch, J.E. Jackson1, G.J. Blanchard, and M. Dantus, "Isoenergetic Two-Photon Excitation Enhances Solvent-to-Solute Excited-State Proton Transfer," *J. Chem. Phys*., **153**, 224301 (2020).

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

42) 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 (2020).

43) 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 (2021).

44) 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 (2021).

45) 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*., published online, e1966534 (2021) DOI: 10.1080/00268976.2021.1966534

46) 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 (2021).

47) 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*., in revision (2021).

48) J. Shen and P. Piecuch, "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(*P*;*Q*) Methodology: Extension to Excited State and Application to Potential Cuts of Water," in preparation.

49) J. Shen and P. Piecuch, "Performance of the CC(t;3) Method, Excited State Potential Energy Surfaces of CH^+," in preparation.

Conference Presentations

Invited talk:

J. Shen and S. Li, "Block-correlated Coupled-Cluster Method with a CASSCF Wave Function: Applications for Low-Lying Electronic Excited States," An International Symposium "Recent Advances in Many Electron Theories," Shankarpur, West Bengal, India, January 5-7, 2010.

Poster Presentations Given by Jun Shen:

1) 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.

2) 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.

3) 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.

4) 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.

5) J. Shen and P. Piecuch, "Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies," American Conference on Theoretical Chemistry, Telluride, Colorado, U.S.A., July 20-25, 2014.

6) Jun Shen, N.P. Bauman, and Piotr Piecuch, "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(P;Q) Methodology: Ground and Excited States" 2015 Midwest Theoretical Chemistry Conference, University of Michigan, Ann Arbor, Michigan, U.S.A., June 26-28, 2015.

7) 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.

8) 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.

9) 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.

Talks and Posters Presented by Co-Authors:

1) S. Li, J. Shen, E. Xu, and Z. Kou, “Advances in coupled cluster methods for bond-breaking potential energy surfaces,” An International Symposium “Recent Advances in Many Electron Theories,” Shankarpur, West Bengal, India, January 5-7, 2010 [invited talk given by S. Li].

2) P. Piecuch, W. Li, J. Shen, J.J. Lutz, and M. W loch, “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].

3) P. Piecuch, W. Li, J. Shen, J.R. Gour, J.J. Lutz, and M. W loch, “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].

4) P. Piecuch, W. Li, J. Shen, J.J. Lutz, J.R. Gour, J.A. Hansen, and M. W loch, “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].

5) P. Piecuch, J. Shen, M. W loch, 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].

6) P. Piecuch, J. Shen, W. Li, J.J. Lutz, M. W loch, 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 on Many Electron Theories II, 2011,” Puri, Orissa, India, December 1-4, 2011 [invited talk given by P. Piecuch].

7) 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].

8) P. Piecuch, J. Shen, W. Li, J.R. Gour, J.J. Lutz, M. W loch, J.A. Hansen, and N.P. Bauman, "Recent Progress in Renormalized and Active-Space Coupled-Cluster Methods," "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].

9) 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].

10) 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].

11) 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].

12) 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].

13) 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].

14) 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].

15) 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].

16) 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 [invited talk given by P. Piecuch].

17) J. Shen, N.P. Bauman, and P. Piecuch, "Combining Active-Space Coupled-Cluster Approaches 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].

18) 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," American Conference on Theoretical Chemistry, Telluride, Colorado, U.S.A., July 20-25, 2014 [poster presented by N.P. Bauman].

19) 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].

20) 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].

21) 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].

22) 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 (TCS2014), Pune, India, December 18-21, 2014 [invited keynote lecture given by P. Piecuch].

23) 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].

24) 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].

25) 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].

26) 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].

27) 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].

28) 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].

29) 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 Be2," 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].

30) 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].

31) 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].

32) 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].

33) 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].

34) 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].

35) 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].

36) 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].

37) 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].

38) 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].

39) 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 to be presented by A.O. Ajala].

40) 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].

41) 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].

42) 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].

43) 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].

44) 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].

45) 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].

46) 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].

47) 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].

48) 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].

49) 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].

50) 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].

51) 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].

52) 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].

53) P. Piecuch, J.E. Deustua, and J. Shen, “New Paradigm in Quantum Chemistry: Accurate Electronic Energies by a Combination of 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].

54) 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].

55) 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].

56) 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].

57) 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 Theoretic Chemistry" (CTTC VIII), Cracow, Poland, September 1-4, 2019 [invited talk given by P. Piecuch].

58) 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].

59) 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].

60) 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].

61) 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].

62) 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].

63) 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].

64) 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].

65) 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 Developments in Coupled-Cluster Theory," Telluride, Colorado, U.S.A., July 19-23, 2021 [hybrid format; invited talk given by P. Piecuch via Zoom].