LIST OF PUBLICATIONS

1. Monographs, Book Chapters, and Feature Articles††


† 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.


2. Articles


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).


honor of Professor Henry F. Schaefer, III; edited by T.D. Crawford and C.D. Sher-rell; invited contribution].


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


† Excluding memberships of editorial boards, which are listed in section Editorial Boards of Curriculum Vitae.
LIST OF INVITED TALKS AT NATIONAL AND INTERNATIONAL SYMPOSIA†


† 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.


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].


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.


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].


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.


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.

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.


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.


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.


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.


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.


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].

In addition, Dr. Piotr Piecuch has been invited to present a 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].


† 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.


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.


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].


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.


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.


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.


Investigaciones Científicas (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.


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.


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 Wroclaw, Wroclaw, Poland, October 11, 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.


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.


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.


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, Louisville, Kentucky, March 7, 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.


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.


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.


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 Molec-
ular 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 Elec-
tronic Excitations in Radicals and Biradicals via Renormalized and Active-Space Coupled-
Cluster Theories, their Merger, and Open-Shell Extensions,” The symposium on Com-
bustion Chemistry, 245th American Chemical Society National Meeting, New Orleans,
Louisiana, 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: Method-
ology,” 245th American Chemical Society National Meeting, New Orleans, Louisiana,
U.S.A., April 7-11, 2013.

171. **“The Cobalt-Methyl Dissociation and Electronic Transitions in Methylcobalamin: In-
sights from the Coupled-cluster, Multireference Perturbation Theory, and Density Func-
tional Theory Calculations,” The symposium “Bioinorganic Chemistry: Proteins and Enzymes and Model Systems,” 245th American Chemical Society National Meeting,

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: In-
sights from Coupled-Cluster, Multireference Perturbation Theory, and Density Func-
tional 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 War-
saw, 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 The-

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 Molec-
ular Systems,” Faculty of Chemistry, Jagiellonian University, Cracow, Poland, Septem-
ber 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, Wroclaw University of Technology, Wroclaw, Poland, September 9, 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.


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 (TCS2014), Pune, India, December 18-21, 2014 [invited keynote lecture].


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, U.S.A., September 24, 2015.


202.** "Coupled-Cluster Interpretation of the Photoelectron Spectra of Ag₃⁻ and Au₃⁻," 26th Austin Symposium on Molecular Structure and Dynamics, Dallas, Texas, U.S.A., March 5-7, 2016.


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


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.


“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].


“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.


TBD, Workshop on New Methods for Strongly Correlated Electrons, Qingdao, China, October 9-13, 2019.

TBD, The Xingda Lectureship, College of Chemistry and Molecular Engineering, Peking University, Beijing, China, November 15, 2019.


TBD, Department of Chemistry, University of Cambridge, March 4, 2020.


In addition, Dr. Piotr Piecuch has been invited to present a 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†


† 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 **.


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 XR + h\nu \rightarrow [M^* \cdot XR]^\dagger \rightarrow \left[M^+ \cdots XR^-\right]^\dagger \rightarrow \text{products (X = F, Cl, Br; R = H, CH}_3,\text{)},” 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].


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,

57. R. Burcl, P. Piecuch, V. Špirko, and O. Bludský, “Bound and Quasi-Bound States of
the Li···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··XR + hν → [M*··XR]‡ →
[M⁺··XR−]‡ → products: Results for M = Li, X = F, R = H, CH₃,” 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].

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

60. P. Piecuch, “Dynamics of Photo-Induced Charge Transfer in van der Waals Molecules,”
Joint Polish-German Conference on Modern Optics: Fundamental Aspects of Spec-
troscopy and Environmental Applications, Jurata near Gdánsk, 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···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···FCH₃ 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].

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].

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].


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].


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].


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].


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


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].


189.** P. Piecuch, M. Wloch, 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].


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].


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].

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 Excita-
tion 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].

Advances in Renormalized and Active-Space Coupled-Cluster Methods,” The sympos-
ium “Reduced Density Matrices in Quantum Chemistry,” 242nd American Chemical
[invited talk given by P. Piecuch].

225.∗∗ P. Piecuch and W. Li, “Local Coupled-Cluster Methods for Chemical Reaction Path-
ways 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].

tation 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 Path-
ways 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].

Supermolecular Strategies in Evaluating the Hydrogen-Bonding-Induced Shifts of Excita-
tion Energies,” Fall 2011 Meeting and General Assembly of the Swiss Chemical Society,
Lausanne, Switzerland, September 9, 2011 [poster presented by G. Fradelos].


255.** J.A. Hansen, M. Ehara, and P. Piecuch, “Aerobic Oxidation of Methanol on Au8− 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].


J. Shen, N.P. Bauman, and P. Piecuch, “Combining Active-Space Coupled-Cluster Methods with Moment Energy Corrections via the \( \text{CC}(P;Q) \) 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


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,


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


328.** TBD, The Utah Workshop on Quantum Methods in Molecular and Solid-State Theory, Park City, Utah, U.S.A., September 22-27, 2019 [invited talk to be given by P. Piecuch].

329.** TBD, Workshop on New Methods for Strongly Correlated Electrons, Qingdao, China, October 9-13, 2019 [invited talk to be given by P. Piecuch].


331.** TBD, The 2020 American Conference on Theoretical Chemistry (ACTC 2020), Squaw Valley, California, U.S.A., July 26-30, 2020 [invited talk to be given by P. Piecuch].

332.** TBD, Twelfth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2020), Vancouver, British Columbia, Canada, August 16-21, 2020 [invited talk to be given by P. Piecuch].