

# Curriculum Vitae

Marta Wloch, Ph.D.

## 1. Biographical data

- a. Name: Marta Wloch  
b. Department: Chemistry  
c. Rank: Assistant Professor

## 2. Education

Ph.D.	University of Silesia, Katowice, Poland	2004	Chemistry
M.Sc.	University of Silesia, Katowice, Poland	1999	Chemistry

## 3. Professional experience

### *a. Teaching experience not as a graduate student:*

Oakland University	Assistant Professor	2011 – present	(Full Time)
Michigan Technological University	Assistant Professor	2007 – 2011	(Full Time)
II High School, Katowice, Poland	Chemistry Teacher	1999 – 2001	(Part Time)

### *b. Teaching experience as a graduate student:*

University of Silesia, Katowice, Poland	Teaching Assistant	1999-2002
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### *c. Other relevant professional experience:*

Michigan State University	Research Assistant Professor	2006 – 2007
Michigan State University	Postdoctoral Research Associate	2004 – 2006
Ames Laboratory, Iowa State University	Visiting Scientist	April 2005
Quantum Theory Project, University of Florida	Visiting Scientist	March-May 2001

*d. Workshops attended:*

- Workshop, "Computational Chemistry for Chemistry Educators", NSF, San Jose, California, USA, (August 1, 2010 - August 7, 2010).
- Workshop, "Theoretical and Computational Chemistry for Chemistry Educators", NSF, Salt Lake City, Utah, USA, (June 12, 2011 - June 17, 2011).

*e. Oakland instructional record (evaluations available for all courses listed below):*

<i>Semester and Year</i>	<i>Course</i>	<i>Enrollment</i>	<i>Evaluations Available?</i>
Fall 2011	CHM 157/143 General Chemistry I	148	Yes
Winter 2012	CHM 541 Advanced Physical Chemistry	2	No
Fall 2012	CHM 157/143 General Chemistry I	150	Yes
Winter 2013	SCI 100 Physical Science in Life, the World, and Beyond	64	No
Fall 2013	CHM 343 Physical Chemistry II	36	Yes
Winter 2014	CHM 157/143 General Chemistry I	136	Yes
Fall 2014	CHM 144/143 General Chemistry I	108	Yes
Winter 2015	CHM 348 Physical Chemistry Lab	16	Yes
Fall 2015	CHM 343 Physical Chemistry II	43	Yes
Winter 2016	CHM 348 Physical Chemistry Lab	16	Yes
Fall 2016	CHM 541 Advanced Physical Chemistry	13	Yes
Winter 2017	CHM 348 Physical Chemistry Lab	12	Yes

**4. Research, Scholarship, Publications, and related activities**

*a. Doctoral dissertation:*

"Electronic excited states based on the coupled-cluster method with full inclusion of the triple excitations"

*b. Master's thesis:*

"Equation-of-motion coupled- cluster method with full inclusion of the triple excitations "

*c. Book published or in press:*

1. Piotr Piecuch, Marta Wloch, Jeffrey R. Gour, Wei Li, and Jesse 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)*, Vol. 1642, edited by T.E. Simos and G. Maroulis, (American Institute of Physics, Melville, NY, 2015), pp. 172-175.
2. Georgios Fradelos, Jesse J. Lutz, Tomasz A. Wesolowski, Piotr Piecuch, Marta Wloch, "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. Brandas, J. Maruani, P. Piecuch, and G. Delgado-Barrio, (Springer, Dordrecht, 2012), pp. 219-248.
3. Piotr Piecuch, Marta Wloch, Antonio 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, edited by S. Lahmar, J. Maruani, S. Wilson and G.Delgado-Barrio, (Springer, Berlin, 2007), pp. 63-121.
4. Piotr Piecuch, Marta Wloch, Maricris D. Lodriguito, Jeffrey R. Gour, "Noniterative coupled-cluster methods for excited electronic states", in: *Progress in Theoretical Chemistry and Physics*, Vol. 15, edited by J. P. Julien, J. Maruani, D. Mayou, S. Wilson, G. Delgado-Barrio, (Springer, Berlin, 2006), pp. 45-106.
5. David J. Dean, Morten Hjorth-Jensen, Karol Kowalski, Piotr Piecuch, Marta Wloch, "Coupled cluster theory for nuclei", in: *Condensed Matter Theories*, Vol. 20, edited by J. W. Clark, R.M. Panoff, and H. Li, (Nova Publishers, 2006), pp. 89-97.
6. David J. Dean, Morten Hjorth-Jensen, Karol Kowalski, Thomas Papenbrock, Marta Wloch, Piotr 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.
7. Piotr Piecuch, Marta Wloch, Jeffrey R. Gour, David J. Dean, Morten Hjorth-Jensen, Thomas Papenbrock, "Bridging quantum chemistry and nuclear structure theory: Coupled-cluster calculations for closed- and open-shell nuclei", in: *Nuclei and Mesoscopic Physics*, Vol. 777, edited by V. Zelevinsky, (AIP Press, 2005), pp. 28-45.

*d. Articles published or in press (peer reviewed journal articles only):*

1. Nina Tymińska, Marta Wloch, A. Timothy Royappa, "Mind the Correct Basis Set: A Case Study for Predicting Gas Phase Acidities of Small Compounds Using Calculations from First Principles", *Int. J. Quantum Chem.* with the front cover art, 115, 42, (2015).
2. Georgios Fradelos, Jesse J. Lutz, Tomasz A. Wesolowski, Piotr Piecuch, Marta Wloch, "Embedding vs Supermolecular Strategies in Evaluating the Hydrogen-Bonding-Induced Shifts of Excitation Energies," *J. Chem. Theory Comput.* 7, 1647 (2011).
3. Jeffrey R. Gour, Piotr Piecuch, Marta Wloch, "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 (2010).
4. Piotr Piecuch, Jeffrey R. Gour, Marta Wloch, "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 (2009).
5. Yingbin Ge, Mark Gordon, Piotr Piecuch, Marta Wloch, Jeffrey 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 (2008).
6. Christopher J. Cramer, Jeffrey R. Gour, Armagan Kinal, Marta Wloch, Piotr Piecuch, Abdul Rehaman Moughal Shahi, Laura Gagliardi, "Stereochemical effects on molecular geometries and state-energy splittings of ligated monocopper dioxygen complexes", *J. Phys. Chem. A*, 112, 3754 (2008).
  7. Piotr Piecuch, Jeffrey R. Gour, Marta Wloch, "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 (2008).
  8. Jingjing Zheng, Jeffrey R. Gour, Jesse J. Lutz, Marta Wloch, Piotr Piecuch, Donald G. Truhlar, "A comparative assessment of the perturbative and renormalized coupled cluster theories with a noniterative treatment of triple excitations for thermochemical kinetics, including a study of basis set and core correlation effects", *J. Chem. Phys.*, 128, 044108 (2008).
  9. Piotr Piecuch, Marta Wloch, Antonio J.C. Varandas, "Application of renormalized coupled-cluster methods to potential function of water", *Theor. Chem. Acc.*, 120, 59 (2008).
  10. Marta Wloch, Jeffrey R. Gour, Piotr 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 (2007).
  11. Gaute Hagen, Thomas Papenbrock, David J. Dean, Achim Shwenk, Andreas Nogga, Marta Wloch, Piotr Piecuch, "Coupled-cluster theory for three-body Hamiltonians", *Phys. Rev. C*, 76, 034302 (2007).
  12. Mihai Horoi, Jeffrey R. Gour, Marta Wloch, Maricris D. Lodriguito, B. Alex Brown, Piotr Piecuch, "Coupled-cluster and configuration-interaction calculations for heavy nuclei", *Phys. Rev. Lett.*, 98, 112501 (2007).
  13. Thomas Papenbrock, David J. Dean, Jeffrey R. Gour, Gaute Hagen, Morten Hjorth-Jensen, Piotr Piecuch, Marta Wloch, "Coupled-cluster theory for nuclei", *Int. J. Mod. Phys. B*, 20, 5338 (2006).
  14. Christopher J. Cramer, Armagan Kinal, Marta Wloch, Piotr Piecuch, Laura Gagliardi, "Theoretical characterization of end-on and side-on peroxide coordination in ligated  $\text{Cu}_2\text{O}_2$  models", *J. Phys. Chem. A*, 110, 11557 (2006).
  15. S. Coussan, Y. Ferro, A. Trivella, P. Roubin, R. Wieczorek, C. Manca, P. Piecuch, K. Kowalski, M. Wloch, S.A. Kucharski, M. Musial, "Experimental and theoretical UV characterizations of acetylacetone and its isomers", *J. Phys. Chem. A*, 110, 3920 (2006).
  16. Christopher J. Cramer, Marta Wloch, Piotr Piecuch, Cristina Puzzarini, Laura Gagliardi, "Theoretical models on the  $\text{Cu}_2\text{O}_2$  torture track. Mechanistic implications for oxytyrosinase and small-molecule analogs", *J. Phys. Chem. A*, 110, 1991 (2006).
  17. Marta Wloch, Maricris D. Lodriguito, Piotr Piecuch, Jeffrey R. Gour, "Two new classes of noniterative coupled-cluster methods derived from the method of moments of coupled-cluster equations", *Mol. Phys.*, 104, 2149 (2006).
  18. Jeffrey R. Gour, Piotr Piecuch, Morten Hjorth-Jensen, Marta Wloch, David J. Dean, "Coupled-cluster calculations for valence systems around  $^{16}\text{O}$ ", *Phys. Rev. C*, 74, 024310 (2006).
  19. Jeffrey R. Gour, Piotr Piecuch, Marta Wloch, "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 (2006).
  20. Maricris D. Lodriguito, Karol Kowalski, Marta Wloch, Piotr Piecuch, "Noniterative coupled-cluster methods employing multi-reference perturbation theory wave functions", *J. Mol. Struct. THEOCHEM*, 771, 89 (2006).
  21. Piotr Piecuch, Marta Wloch, Jeffrey R. Gour, Armagan Kinal, "Single-reference, size-extensive, non-iterative coupled-cluster approach to bond breaking and biradicals", *Chem. Phys. Lett.*, 418, 467 (2006).
  22. Piotr Piecuch, Marta Wloch, "Renormalized coupled-cluster methods exploiting left eigenstates of the similarity-transformed Hamiltonian", *J. Chem. Phys.*, 123, 224105 (2005).

23. Marta Wloch, David J. Dean, Jeffrey R. Gour, Piotr Piecuch, Morten Hjorth-Jensen, Thomas Papenbrock, Karol Kowalski, "Ab initio coupled cluster calculations for nuclei using methods of quantum chemistry", *Eur. Phys. J. A*, 25, 485 (2005).
24. David J. Dean, Jeffrey R. Gour, Gaute Hagen, Morten Hjorth-Jensen, Karol Kowalski, Thomas Papenbrock, Piotr Piecuch, Marta Wloch, "Nuclear structure calculations with coupled cluster methods from quantum chemistry", *Nucl. Phys. A*, 752, 299 (2005).
25. Marta Wloch, David J. Dean, Jeffrey R. Gour, Morten Hjorth-Jensen, Karol Kowalski, Thomas Papenbrock, Piotr Piecuch, "Ab-initio coupled-cluster study of  $^{16}\text{O}$ ", *Phys. Rev. Lett.*, 94, 212501 (2005).
26. Marta Wloch, Jeffrey R. Gour, Piotr Piecuch, David J. Dean, Morten Hjorth-Jensen, Thomas 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, 1291 (2005).
27. Jeffrey R. Gour, Piotr Piecuch, Marta Wloch, "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 (2005).
28. Karol Kowalski, So Hirata, Marta Wloch, Piotr Piecuch, Theresa L. Windus, "Active-space coupled-cluster study of electronic states of  $\text{Be}_3$ ", *J. Chem. Phys.*, 123, 074319 (2005).
29. Marta Wloch, Jeffrey R. Gour, Karol Kowalski, Piotr Piecuch, "Extension of renormalized coupled-cluster methods including triple excitations to excited electronic states of open-shell molecules", *J. Chem. Phys.*, 122, 214107 (2005).
30. Rajat K. Chaudhuri, Karl F. Freed, Gabriel Hose, Piotr Piecuch, Karol Kowalski, Marta Wloch, Sudip Chattopadhyay, Debashis Mukherjee, Zoltan Rolik, Agnes Szabados, Gabor Toth, Peter R. Surjan, "Comparison of low-order multireference many-body perturbation theories", *J. Chem. Phys.*, 122, 134105 (2005).
31. Marta Wloch, Monika Musial, Stanislaw A. Kucharski, "Connected triple excitations in the equation-of-motion coupled cluster calculations of the energies and properties of excited states: HCN molecule", *Comput. Met. Sci. Tech.*, 9, 163 (2003).
32. Marta Wloch, Stanislaw A. Kucharski, "Approximate ground state wave function in the full EOMCCSDT calculations", *Annals of Pol. Chem. Soc.*, 2, 918 (2003).
33. Marta Wloch, Monika Musial, Stanislaw A. Kucharski, "Equation-of-motion coupled-cluster method with full inclusion of the triple excitations", *Annals of Pol. Chem. Soc.*, 1, 255 (2001).
34. Stanislaw A. Kucharski, Marta Wloch, Monika Musial, Rodney J. Bartlett, "Coupled cluster theory for excited electronic states: the full EOM-CCSDT method", *J. Chem. Phys.*, 115, 8263 (2001).

*e. Oral presentation; performances; exhibitions (presenter underlined, PI indicated by \*):*

### **Invited Lectures**

1. "Computational Chemistry and the Art of Compromise", Oakland University, Rochester, Michigan, USA, 18th November 2015.
2. "Highly Accurate but Easy-to-Use Computational Methods", Wayne State University, Detroit, Michigan, USA, 28th January 2015.
3. "New Methods and Software Development for Many Fermions Systems. Applications in Chemistry and Nuclear Physics", Oakland University, Rochester, Michigan, USA, 17th January 2010.
4. "New Methods and Software Development for Many Fermions Systems", EMSL, Pacific Northwest National Laboratory, Richland, Washington, USA, 9th October 2009.

5. "Recent Developments and Applications of the Renormalized Coupled-Cluster Methods", Canadian Society for Chemistry Symposium on Static Electron Correlation (CSC 2009), Hamilton, Ontario, Canada, 1st June 2009.
6. "Recent Developments and Applications of the Renormalized Coupled-Cluster Methods", Thirteenth International Workshop on Quantum Systems in Chemistry and Physics (QSCP-XIII), East Lansing, Michigan, USA, 8th July 2008.
7. "Accurate Quantum Calculations for Many-Body Systems", House/Rekhi presentation as part of computing initiative proposal, Michigan Technological University, Houghton, Michigan, USA, 25th March 2008.
8. "Renormalized Coupled-Cluster Approaches: Practical Computational Tools for Accurate Studies of Bond Breaking, Biradicals, and Excited Electronic States", Michigan Technological University, Houghton, Michigan, USA, 13th December 2006.
9. "Renormalized Coupled-Cluster Approaches: Practical Computational Tools for Accurate Studies of Bond Breaking, Biradicals, and Excited Electronic States", Ball State University, Muncie, Indiana, USA, 11th December 2006.
10. "Renormalized Coupled-Cluster Approaches: Practical Computational Tools for Accurate Studies of Bond Breaking, Biradicals, and Excited Electronic States", California State University - Long Beach, Long Beach, California, USA, 28th November 2006.
11. "Nuclear Shell Model Applications", School on Tools and Toys of Nuclear Astrophysics, The Joint Institute for Nuclear Astrophysics, Michigan State University, East Lansing, Michigan, USA, 14th February 2006.
12. "Large-scale ab initio quantum calculations for molecules, radicals, and atomic nuclei using HPCC computer system", HPCC Open House/Symposium, Michigan State University, East Lansing, Michigan, USA, 8th October 2005.
13. "The open-shell extension of the renormalized equation of motion coupled-cluster method and its applications to many-electron and other many-fermion systems", Ames Laboratory/Iowa State University, Ames, Iowa, USA, 19th April 2005.
14. "Coupled-cluster equation-of-motion method with full inclusion of the connected triple excitations", Quantum Theory Project, University of Florida, Gainesville, Florida, USA, 4th April 2001.

## Conference Presentations

1. Marta Wloch, Piotr Piecuch, Jeffrey R. Gour, "Recent Developments and Applications of the Renormalized Coupled-Cluster Methods", Canadian Society for Chemistry Symposium on Static Electron Correlation (CSC 2009), Hamilton, Ontario, Canada, 30 May-3 June 2009.
2. Marta Wloch, Piotr Piecuch, Jeffrey R. Gour, "Recent Developments and Applications of the Renormalized Coupled-Cluster Methods", Thirteenth International Workshop on Quantum Systems in Chemistry and Physics (QSCP-XIII), East Lansing, Michigan, USA, 6-12 July 2008.
3. Marta Wloch, Armagan Kinal, Jeffrey R. Gour, Piotr Piecuch, "Single-reference, size-extensive, non-iterative coupled-cluster approaches to bond breaking and biradicals", XIIth International Congress of Quantum Chemistry, Kyoto, Japan, 21-26 May 2006.
4. Marta Wloch, Piotr Piecuch, "Extension of renormalized coupled-cluster methods including triple excitations to ground and excited electronic states of open-shell molecules", XIIth International Congress of Quantum Chemistry, Kyoto, Japan, 21-26 May 2006.
5. Marta Wloch, Jeffrey R. Gour, Piotr 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, New Orleans, Louisiana, USA, 20-26 July 2005.
6. Marta Wloch, Piotr 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”, 45th Sanibel Symposium, St. Simons Island, Georgia, USA, 5-11 March 2005.
7. Karol Kowalski, Marta Wloch, Piotr Piecuch, ”Efficient implementation of the standard and renormalized equation of motion coupled-cluster methods in GAMESS”, 36th Midwest Theoretical Chemistry Conference, East Lansing, Michigan, USA, 17-19 June 2004.
  8. Marta Wloch, Stanislaw A. Kucharski ”Electronic excitations energies based on the coupled cluster method with full inclusion of the connected triple excitations”, Central European Symposium on Theoretical Chemistry, Nove Hradý, Czech Republic, 25-28 September 2003.
  9. Marta Wloch, Stanislaw A. Kucharski ”Electronic excitations energies based on the coupled cluster method with full inclusion of the connected triple excitations” XLVI PTChem and SITPChem Meeting, Lublin, Poland, 15-18 September 2003.
  10. Marta Wloch, Stanislaw A. Kucharski ”The triple excitation corrections in coupled cluster theory for excited electronic states: the full EOM-CCSDT method.”, 1st Central European Symposium on Theoretical Chemistry, Zwettl, Austria, 28-30 October 2002.
  11. Marta Wloch, Stanislaw A. Kucharski, Rodney J. Bartlett, ”Coupled-cluster theory for excited electronic states with full inclusion of the triple excitations: EOM-CCSDT method”, Austrian-Czech-Polish-Slovak Symposium on Quantum Chemistry, Ustroń-Jaszowiec, Poland, 27-30 September 2001.
  12. Marta Wloch, Stanislaw A. Kucharski ”Excited states of the molecules in the computations including  $T_3$  operator”, XLIV PTChem and SITPChem Meeting, Katowice, Poland, 9-13 September 2001.
  13. Marta Wloch, Stanislaw A. Kucharski ”The EOM method based on the CCSDT model of the coupled-cluster theory.” PTChem and SITPChem Meeting, Lodz, Poland, 10-15 September 2000.
  14. Marta Wloch, Stanislaw A. Kucharski ”Coupled-cluster equation-of-motion method with full inclusion of the connected triple excitations”, Third European Conference on Computational Chemistry, Budapest, Hungary, 4-8 September 2000.

### Talks and Posters Presented at Conferences by Co-authors

1. P. Piecuch\*, K. Kowalski, D.J. Dean, M. Hjorth-Jensen, T. Papenbrock, and M. Wloch, ”Coupled Cluster Calculations of Ground and Excited States of Nuclei”, International Conference on Exotic Nuclei and Atomic Masses, ENAM-04, Pine Mountain, Georgia, USA, September 12-16, 2004.
2. P. Piecuch\*, K. Kowalski, M. Wloch, 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.
3. P. Piecuch\*, M. Wloch, 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.
4. P. Piecuch\*, K. Kowalski, M. Wloch, 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.
5. D.J. Dean\*, J.R. Gour, G. Hagen, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock, P. Piecuch, and M. Wloch, ”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.

6. M.D. Lodrigo, K. Kowalski, M. Wloch, 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, USA, March 5-11, 2005 [poster].
7. P. Piecuch\*, M. Wloch, 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 (ICTCPV), New Orleans, Louisiana, USA, July 20-26, 2005.
8. J.R. Gour, M. Wloch, 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, USA, July 20-26, 2005 [poster].
9. S. Coussan, A. Trivella, C. Manca, Y. Ferro, M. Rajzmann, R. Wieczorek, P. Piecuch, K. Kowalski, M. Wloch, S.A. Kucharski, M. Musia l, 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.
10. P. Piecuch\*, M. Wloch, J.R. Gour, K. Kowalski, A. Kinal, M. Lodrigo, 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, USA, August 28-September 1, 2005.
11. P. Piecuch\*, M. Wloch, 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.
12. P. Piecuch\*, J.R. Gour, M. Wloch, 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.
13. P. Piecuch\*, M. Wloch, 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].
14. P. Piecuch\*, M. Wloch, J.R. Gour, and A. Kinal, "Advances in electronic structure theory: single-reference methods for multi-reference problems", XIIth International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006.
15. P. Piecuch\*, M. Wloch, J. R. Gour, D. J. Dean, T. Papenbrock, M. Hjorth-Jensen, "Bridging quantum chemistry and nuclear structure theory: Coupled-cluster calculations for closed- and open-shell nuclei", XIIth International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [poster].
16. J. R. Gour, P. Piecuch\*, M. Wloch, "Active-space equation-of-motion coupled-cluster methods for ground and excited states of radicals", XIIth International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [poster].
17. A. Kinal, M. J. McGuire, M. Wloch, and P. Piecuch\*, " Completely renormalized coupled-cluster and MRCI studies of the thermal stereomutations of cyclopropane", 38th Midwest Chemistry Conference, Columbus, Ohio, USA, June 15-17, 2006.
18. M. D. Lodrigo, M. Wloch, and P. Piecuch\*, "Non-iterative coupled-cluster methods employing multireference perturbation theory wave functions", 38th Midwest Chemistry Conference,



- Columbus, Ohio, USA, June 15-17, 2006 [poster].
19. P. Piecuch\*, M. Wloch, 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, Canada, July 26-30, 2006.
  20. M. D. Lodriguito, M. Wloch, and P. Piecuch\*, "Non-iterative coupled-cluster methods employing multi-reference perturbation theory wave functions", Sixth Canadian Computational Chemistry Conference (CCCC6), Vancouver, Canada, July 26-30, 2006 [poster].
  21. P. Piecuch\*, M. Wloch, 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.
  22. P. Piecuch\*, M. Wloch, 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].
  23. P. Piecuch\*, J.R. Gour, and M. Wloch, "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].
  24. P. Piecuch\*, M. Wloch, 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.
  25. P. Piecuch\*, J.R. Gour, and M. Wloch, "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, USA, January 15-18, 2007.
  26. M. Horoi, J.R. Gour, M. Wloch, M.D. Lodriguito, P. Piecuch, and B.A. Brown\*, "Coupled-Cluster and Configuration-Interaction Calculations for Heavy Nuclei", Session X16, "Nuclear Theory II", 2007 American Physical Society April Meeting, Jacksonville, Florida, USA, April 14-17, 2007.
  27. P. Piecuch\*, M. Wloch, 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, USA, June 28-30, 2007.
  28. P. Piecuch\*, M. Wloch, 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.
  29. P. Piecuch\*, M. Wloch, 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", Wroclaw/Ladek-Zdroj, Poland, September 13-18, 2007.
  30. J.R. Gour, M. Wloch, 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, USA, October 20-22, 2007 [poster].
  31. J.R. Gour, P. Piecuch\*, and M. Wloch, "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, USA, October 20-22,

- 2007 [poster].
32. M. Wloch, 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, USA, October 20-22, 2007 [poster].
  33. Y. Ge, M.S. Gordon\*, P. Piecuch, M. Wloch, 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, USA, April 6-10, 2008.
  34. P. Piecuch\*, M. Wloch, 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, USA, April 6-10, 2008.
  35. J.R. Gour, M. Wloch, 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 (QSCP-XIII), East Lansing, Michigan, USA, July 6-12, 2008 [poster].
  36. P. Piecuch\*, M. Wloch, J.R. Gour, and Wei 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.
  37. P. Piecuch\*, M. Wloch, J.R. Gour, Wei 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.
  38. P. Piecuch\*, Wei Li, J.R. Gour, and M. Wloch, "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems", The International Conference on Theory and Applications of Computational Chemistry 2008 (TACC 2008), Shanghai, China, September 23-27, 2008.
  39. P. Piecuch\*, J.R. Gour, Wei Li, M. Wloch, 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, USA, August 16-20, 2009.
  40. P. Piecuch\*, J.R. Gour, W. Li, M. Wloch, 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.
  41. P. Piecuch\*, J.R. Gour, M. Wloch, J.J. Lutz, and Wei 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.
  42. P. Piecuch\*, M. Wloch, 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 Cizek and Josef Paldus, Kos, Greece, October 3-8, 2010.

43. J.J. Lutz, G. Fradelos, T.A. Wesolowski, P. Piecuch\*, and M. Wloch, "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].
44. P. Piecuch\*, W. Li, J. Shen, J.J. Lutz, and M. Wloch, "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.
45. J.J. Lutz, G. Fradelos, T.A. Wesolowski, P. Piecuch\*, and M. Wloch, "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.
46. P. Piecuch\*, W. Li, J. Shen, J.R. Gour, J.J. Lutz, and M. Wloch, "Recent Advances in Renormalized and Active-Space Coupled-Cluster Methods," WATOC 2011 Satellite Conference "Strongly Correlated Systems, Cooperativity, and Valence-Bond Theory," A Coruna, Spain, July 23-24, 2011.
47. P. Piecuch\*, W. Li, J. Shen, J.J. Lutz, J.R. Gour, J.A. Hansen, and M. Wloch, "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.
48. P. Piecuch\*, G. Fradelos, J.J. Lutz, T.A. Wesolowski, and M. Wloch, "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.
49. G. Fradelos, J.J. Lutz, T.A. Wesolowski\*, P. Piecuch, and M. Wloch, "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].
50. P. Piecuch\*, J. Shen, M. Wloch, 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.
51. P. Piecuch\*, J. Shen, W. Li, J.J. Lutz, M. Wloch, 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.
52. Nina Tyminska, Marta Wloch\*: "Theoretical investigation of lithium monoxide anion acidity" – 43rd ACS Central Regional Meeting, Dearborn, Michigan, June 5-9, 2012.
53. P. Piecuch\*, J. Shen, W. Li, J.R. Gour, J.J. Lutz, M. Wloch, 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.

*f. Book reviews:* (none)

*g. Abstracts published or in press (PI indicated by \*):*

*h. Research in progress*

I am working on increasing functionality of my CR-CC(2,3) method. The method works perfect for single point energy computations but the procedure of finding optimized molecular geometry and vibrational frequencies needs further investigation. The other problem which needs to be addressed is the lack of extensivity of the recently developed extension of the CR-CC(2,3) to excited states. I am working on reformulating the CR-CC(2,3) method such that its excited state extension is size extensive.

In the application part of my work, I continue the investigation of metal-dioxygen complexes. A proper description of the bonding interactions in such systems is important to the understanding of the biochemical uptake of oxygen, the synthesis of oxygen-containing organic molecules, and catalytic processes which utilize dioxygen complexation. It is a great challenge to use the appropriate level of theory to answer chemical questions about transition metal complexes and their role in the activation of dioxygen. I am working on automatizing the process of choosing the best lower-order method, such as DFT, for a given large system by analyzing the results from higher-order computations for a model system.

I am also studying the dependence between the positions in the periodic table of the atoms building the molecule and the importance of using different classes of basis sets in computational evaluations of molecular properties.

*i. Grants and contracts:*

i. Current externally funded grants:

ii. Pending externally funded grants:

- “Self-Learning Algorithm for Automation of Large Scale Computations of Bioorganic Molecules” submitted on 9/29/2016 to DOE Office of Science.
- Silicon Mechanics 6th Annual Research Cluster Grant submitted 3/1/2017 in collaboration with professors from physics, biology, and computer science departments (PI: Marta Wloch)

iii. Rejected external grants:

- “REU Site: Summer Undergraduate Multidisciplinary Materials Inspired Training (SUMMIT)” submitted on 8/26/2015 to National Science Foundation in collaboration with professors from physics and biology departments (PI: Yuejian Wang, Physics Department).
- Silicon Mechanics 5th Annual Research Cluster Grant submitted 3/1/2016 in collaboration with professors from physics, biology, and computer science departments (PI: Marta Wloch)
- Silicon Mechanics 4th Annual Research Cluster Grant submitted 3/1/2015 in collaboration with professors from physics, biology, and computer science departments (PI: Yonghong Yan, Department of Computer Science and Engineering).
- “Accurate Computations for Organometallic Systems” submitted on 9/29/2014 to National Science Foundation
- Special Grant Program in the Chemical Sciences submitted 6/3/2013 to The Camille & Henry Dreyfus Foundation
- "Efficient and Accurate Methodology to Study Excited States" submitted on 11/29/2011 to the U.S. Department of Energy (DOE) Office of Science Early Career Research Program

iv. Funded Internal grants:

v. Rejected Internal Grants:

## 5. Public and University Service

### *a. Public Service*

### *b. Professional Service:*

1. Referee of publications submitted to The International Journal of Quantum Chemistry: 2015; The Journal of Physical Chemistry: 2007, 2011; Theoretical Chemistry Accounts: 2008, 2009; The Journal of Chemical Physics: 2009, 2011, 2012(2), 2013, 2014(3), 2015(3); Chemical Physics Letters: 2011
2. Referee of NSF proposal 2008.
3. Referee for Oxford University Press textbooks 2009.
4. Member of the Organizing Committee of the Austrian-Czech-Polish-Slovak Symposium on Quantum Chemistry, Ustron-Jaszowiec, Poland, 27-30 September 2001.
5. Member of the Organizing Committee of the 36th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, USA, 17-19 June, 2004

### *c. University Service:*

1. Marshal at the Graduate Commencement Fall 2011.
2. Faculty Advisor to P.A.T.C.H (Pre-Professional Association towards Careers in Health) since Fall 2013, in April 2014 the organization won the title of Organization of the Year awarded by the Center for Student Activities & Leadership Development at Oakland University.
3. Recommendation/reference letters for the following students (since Fall 2011):
  - Antonio Ndoja - E3S Summer Research Program, University of California, Berkeley; Interdisciplinary Research Experience in Electrical and Computer Engineering, Oakland University
  - Matthew Grant - Eye Research Institute, Oakland University; Undergraduate Summer Research Program, Oakland University; Automotive and Energy Research and Industrial Mentorship Program at Oakland University
  - Wasym Mando - Eye Research Institute, Oakland University; Undergraduate Summer Research Program, Oakland University; Medical School; Michigan State University Graduate School
  - Jason Palmer - Undergraduate Summer Research Program, Oakland University
  - Nicholas Bauman - Michigan State University Graduate School
  - Andrew Kennedy - Michigan Technological University Graduate School
  - Alyssa Venderziel – Medical School, Michigan State University Graduate School
  - Minan Mansour – Medical School
  - Hanna Trzeciakiewicz - A.P.C.S. Scholarship
  - Jessica Koppen - visiting professor position
  - Nadya Al-Hadidi – Pharmacy School
  - Natalia Yono – Pharmacy School
  - Yousif Tolla – Dental School
  - Lydia Gojcevic – Medical School

- Nina Tyminska – Doctoral Finishing Fellowship, postdoctoral position; assistant professor position
- Thu Yen Tran – Medical School

*d. College Service:*

- Kenny Scholarship Selection Committee (Chair: Brad Roth), April 2013

*e. Departmental Service:*

1. Hosting visiting seminar speakers:

Fall 2011			
Piotr Piecuch	Michigan State		Faculty Host
Winter 2012			
Eva Zurek	State University of NY		Faculty Host
Winter 2013			
Dominika Zgid	University of Michigan		Faculty Host
Fall 2013			
Sohail Qamar	DOW/KOKAM		Faculty Host
Yue Qi	General Motors		Faculty Host
Fall 2015			
Konrad Patkowski	Auburn University		Faculty Host

2. Greg Felton C-2 review committee member (FPAC-Services, Chair: Xiangqun Zeng), Fall 2012.
3. PhD thesis committee for Venkata Pottiboyina (Prof. Sevilla's student).
4. PhD thesis committee for Jessica Koppen (Prof. Bryant's student).
5. Wrote/administered cume exam for PhD program, January 2013.
6. Inorganic Faculty Search Committee member (Chair: Michael Sevilla), Fall 2013/Winter 2014
7. David Szlag C-1 review committee member (FPAC-Teaching, Chair: Roman Dembinski), Fall 2014
8. Adjunct Professor Search Committee member (Chair: John Seeley), Fall 2015
9. Graduate Program Committee member (Chair: Xiangqun Zeng), Fall 2015

**Professional Membership:**

American Chemical Society, member

**Students supervised in independent research:**

Nina Tyminska PhD