Curriculum Vitae

Nicholas P. Bauman, Graduate Assistant
Department of Chemistry, Michigan State University
Chemistry Building, 578 S. Shaw Lane, Room 18C
East Lansing, Michigan 48824-1322, USA
Current Mailing Address: 1410 W. Ionia St., Lansing, Michigan 48915
Telephone: (517)353-1156 (work); (586)854-5337 (mobile)
Email: npbauman@chemistry.msu.edu

Education

August 2011 - present, pursuing Ph.D. in theoretical and computational chemistry at Michigan State University, Advisor: Professor Piotr Piecuch

B.S., 2011, Chemistry, Michigan Technological University, Houghton, Michigan, 49931, Concentration: Chemical Physics

Minor, 2011, Mathematical Sciences, Michigan Technological University, Houghton, Michigan, 49931

Minor, 2011, Polymer Science, Michigan Technological University, Houghton, Michigan, 49931

Professional Experience

Michigan State University, August 2011 - present, Graduate Teaching and Research Assistant. Teaching freshman level chemistry and undergraduate physical chemistry courses while performing Ph.D. research in theoretical and computational chemistry. Ph.D. Advisor: Professor Piotr Piecuch.

Michigan Technological University, November 2009 - April 2011, Chemistry Learning Center Coach/Tutor. I tutored undergraduate students in the subject of freshman chemistry, organic chemistry, and physical chemistry.

Research Experience

"Summer Start" and graduate student researcher, May 2011 - present, Michigan State University, Advisor-Professor Piotr Piecuch
My research to date included the examination of the challenging problem of cobalt-methyl dissociation in methylcobalamin with coupled-cluster, density functional theory, and multi-reference methods. The methylcobalamin work resulted in a publication in the *Journal of Chemical Theory and Computation*. My work has also included coupled-cluster, equation-of-motion coupled-cluster, and multi-reference configuration interaction calculations for

cyclobutanetetrone which resulted in a paper in *Molecular Physics*. I have worked on extending the CC(*P*;*Q*) hierarchy of methods to include quadruple excitations. The first paper in this area is in preparation. I have also participated in a collaborative study of species involved in Cu^+-promoted catalysis, in which I performed high-level coupled-cluster calculations in order to establish a benchmark for the evaluation of density functional theory and perturbation theory. The study of these copper species resulted in a paper published in the *Journal of Molecular Modeling*. I have studied the photoelectron spectrum of Au_3^- using the scalar relativistic ionized equation-of-motion coupled-cluster approaches, which resulted in a communication published in the *Journal of Chemical Physics*. Recently, I have applied the same approaches to the photoelectron spectrum of Ag_3^-, and the corresponding paper has been submitted to the *Journal of Chemical Physics*. In addition to the papers mentioned above, these projects have resulted in several posters and talks.

Undergraduate student researcher, 2009-2011, Michigan Technological University
I worked with Professor Marta Włoch. I developed an efficient coupled-cluster singles and doubles program. I also performed several excited-state calculations with the equation-of-motion coupled-cluster methods.

Undergraduate student researcher, Spring 2011, Michigan Technological University
I worked under the supervision of Professor Patricia Heiden studying the moisture barrier properties of block copolymers and the effect of the block structure on these properties.

Undergraduate student researcher, Summer 2009, Michigan Technological University
Thanks to the MTU Chemistry Department's Sandretto-Stackhouse Summer Research Fellowship I worked in Professor Haiying Liu's group where I synthesized several organic compounds and qualitatively analyzed them using various instruments including NMR, UV-Vis Spectrometer, Flourometer, and IR Spectrometer.

Awards

College of Natural Science Summer Dissertation Completion Fellowship, Department of Chemistry, Michigan State University, 2016.

I received a fellowship to attend the Second Annual Software-Development Summer School for Computational Chemistry and Materials Modeling held at Stony Brook University, Stony Brook, NY, July 8-18 2014.

College of Natural Science Summer Dissertation Continuation Fellowship, Department of Chemistry, Michigan State University, 2014.

Education Merit Award for Excellence in Teaching, Michigan State University, 2013-2014 academic year.

Michigan State University Summer Start Fellowship, Department of Chemistry, Michigan State University, 2011. Awarded to incoming graduate students to work in a research lab of a chemistry faculty member of their choosing (Professor Piotr Piecuch).

Leslie Liefer Award in Physical Chemistry, Department of Chemistry, Michigan Technological University, 2011. Awarded to senior undergraduate who has demonstrated excellence and interest in the field of Physical Chemistry.

Outstanding Senior Research Award, Department of Chemistry, Michigan Technological University, 2011. Awarded to the senior undergraduate who is a valuable contributor to faculty research.

Sandretto-Stackhouse Summer Research Fellowship, Department of Chemistry, Michigan Technological University, 2009. Awarded to an undergraduate student to work in a research lab of a chemistry faculty member of their choosing for the summer (Professor Haiying Liu).

Department of Chemistry Ambassador Award, Department of Chemistry, Michigan Technological University, 2008 and 2011. Awarded to the undergraduate students who volunteer their time to promote the Chemistry Department and Michigan Technological University through open houses, family science nights, and other events.

Publications

1. S. Velayundham, C.H. Lee, M. Xie, D. Blair, N. Bauman, Y.K. Yap, S. Green, and H. Liu, "Noncovalent Functionalization of Boron Nitride Nanotubes with Poly(*p*-phenylene-ethynylene)s and Polythiophene," *Appl. Mater. Interfaces* **2**, 104–110 (2010).

2. P.M. Kozłowski, M. Kumar, P. Piecuch, W. Li, N.P. Bauman, J.A. Hansen, P. Lodowski, and M. Jaworska. "The Cobalt-Methyl Bond Dissociation in Methylcobalamin: New Benchmark Analysis Based on Density Functional Theory and Completely Renormalized Coupled-Cluster Calculations," *J. Chem. Theory Comput.* **8**, 1870-1894 (2012).

3. C.E.P. Bernardo, N.P. Bauman, P. Piecuch, and P.J. Silva, "Evaluation of Density Functional Methods on the Geometric and Energetic Descriptions of Species Involved in Cu^{+}-Promoted Catalysis," *J. Mol. Model.* **19**, 5457-5467 (2013).

4. N.P. Bauman, J.A. Hansen, M. Ehara, and P. Piecuch, "Communication: Coupled-Cluster Interpretation of the Photoelectron Spectrum of Au_3^-," *J. Chem. Phys.* **141**, 101102-1 – 101102-5 (2014).

5. 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).

6. N.P. Bauman, J.A. Hansen, and P. Piecuch, "Coupled-Cluster Interpretation of the Photoelectron Spectrum of Ag_3^-," submitted to the *Journal of Chemical Physics.*

7. P. Piecuch, N.P. Bauman, and J. Shen, "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(*P*;*Q*) Methodology: Connected Quadruple Excitations," in preparation for the *Journal of Chemical Physics*.

Contributed Talks Given by Nicholas P. Bauman

1. N.P. Bauman, J.A. Hansen, P. Piecuch, and M. Ehara, "Coupled-Cluster Interpretation of the Photoelectron Spectra of Ag_3^- and Au_3^-," 47th Midwest Theoretical Chemistry Conference, University of Michigan, U.S.A., June 26-28, 2015.

Poster Presentations Given by Nicholas P. Bauman

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

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

3. P.M. Kozłowski, M. Kumar, P. Piecuch, W. Li, N.P. Bauman, J.A. Hansen, P. Lodowski, and M. Jaworska, "The Cobalt-Methyl Bond Dissociation in Methylcobalamin: New Benchmark Analysis Based on Density Functional Theory and Completely Renormalized Coupled-Cluster Calculations," Midwestern Symposium on Undergraduate Research in Chemistry, Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., October 5-6, 2012.

4. P. Piecuch, W. Li, N.P. Bauman, J.A. Hansen, P.M. Kozłowski, M. Kumar, P. Lodowski, and M. Jaworska, "The Cobalt-Methyl Bond Dissociation in Methylcobalamin: New Benchmark Analysis Based on Density Functional Theory and Completely Renormalized Coupled-Cluster Calculations," 45th Midwest Theoretical Chemistry Conference, University of Illinois at Urbana-Champaign, Illinois, U.S.A., May 29-31, 2013.

5. P.M. Kozłowski, M. Kumar, P. Piecuch, W. Li, N.P. Bauman, J.A. Hansen, P. Lodowski, and M. Jaworska, "The Cobalt-Methyl Bond Dissociation in Methylcobalamin: New Benchmark Analysis Based on Density Functional Theory and Completely Renormalized Coupled-Cluster Calculations," Midwestern Symposium on Undergraduate Research in Chemistry, Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., October 4-5, 2013.

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

7. J. Shen, N.P. Bauman, and P. Piecuch, “Combining Active-Space Coupled-Cluster Methods with Moment Energy Corrections via the CC(*P*;*Q*) Methodology, with Benchmark Calculations for Bond Breaking, Transition States, and Singlet-Triplet Gaps in Biradical Systems,” A Symposium on Chemistry and Applications of Advanced Materials in Recognition of Thomas J. Pinnavaia’s 47-year MSU Career, Michigan State University, East Lansing, Michigan, U.S.A., May 10, 2014.

8. N.P. Bauman, J. Shen, and P. Piecuch, “Combining Active-Space Coupled-Cluster Methods with Moment Energy Corrections via the CC(*P*;*Q*) Methodology, Connected Triple and Quadruple Excitations,” The 2014 American Conference on Theoretical Chemistry (ACTC 2014), Telluride, Colorado, U.S.A., July 20-25, 2014.

9. 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.

Talks and Posters Presented by Co-Authors

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

2. 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].

3. P.M. Kozłowski, M. Kumar, P. Piecuch, W. Li, N.P. Bauman, J.A. Hansen, P. Lodowski, and M. Jaworska, “The Cobalt-Methyl Bond Dissociation in Methylcobalamin: New Benchmark Analysis Based on Density Functional Theory and Completely Renormalized Coupled-Cluster Calculations," 14th International Congress of Quantum Chemistry, Boulder, Colorado, U.S.A., June 25-30, 2012 [poster presented by P. Piecuch].

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

5. 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].

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

7. 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].

8. 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].

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

10. P. Piecuch, J. Shen, N.P. Bauman, 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 to be given by P. Piecuch].

11. 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 Chemistry (WATOC 2014), Santiago, Chile, October 5-10, 2014 [invited talk given by P. Piecuch].

12. 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].

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

14. 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].

15. 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].

16. J. Shen, N.P. Bauman, and P. Piecuch, "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(*P*;*Q*) Methodology: Ground and Excited States," 47th Midwest Theoretical Chemistry Conference, University of Michigan, U.S.A., June 26-28, 2015 [poster presented by J. Shen].

17. 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].

18. P. Piecuch, J.A. Hansen, N.P. Bauman, and M. Ehara, "Utility of New Generations of Coupled-Cluster Methods and Algorithms in Catalytic, Structural, and Optical Properties of Gold Nanoparticles," The symposium "Interplay between Theory and Experiment in Catalytic Research," the 2015 International Chemistry Congress of Pacific Basin Societies (Pacifchem 2015), Honolulu, Hawaii, U.S.A., December 15-20, 2015 [invited talk given by P. Piecuch].

19. P. Piecuch, N.P. Bauman, and J.A. Hansen, "Coupled-Cluster Interpretation of the Photoelectron Spectra of Ag_3^- and Au_3^-," 26th Austin Symposium on Molecular Structure and Dynamics, Dallas, Texas, U.S.A., March 5-7, 2016 [invited talk given by P. Piecuch].