

CURRICULUM VITAE

Dr. Piotr Piecuch, University Distinguished Professor
Department of Chemistry, Michigan State University
East Lansing, Michigan 48824-1322, USA*
Telephone: (517) 355 9715, x223; *Fax:* (517) 353 1793

E-mail: piecuch@chemistry.msu.edu; *Internet:* www.cem.msu.edu/~piecuch/group_web

Education

Ph.D., 1988, University of Wrocław, Poland (with Distinction)

M.S., 1983, University of Wrocław, Poland (with Distinction)

Professional Experience

Michigan State University

University Distinguished Professor, Department of Chemistry, Michigan State University, 2007–present

Adjunct Professor, Department of Physics and Astronomy and Member of Nuclear Theory Group at National Superconducting Cyclotron Laboratory, Michigan State University, 2004–present

Professor (with tenure), Department of Chemistry, Michigan State University, 2004–present

Adjunct Associate Professor, Department of Physics and Astronomy, Michigan State University, 2003–2004

Associate Professor (with tenure), Department of Chemistry, Michigan State University, 2002–2004

Assistant Professor (tenure track), Department of Chemistry, Michigan State University, 1998–2002

Other Institutions

Visiting Professor (Professor Catedrático Visitante), Department of Chemistry, University of Coimbra, Portugal, 2006 (3 months)

Visiting Professor, Fukui Institute for Fundamental Chemistry, Kyoto University, Japan, 2005 (2 months)

Adjunct Assistant Professor, Department of Applied Mathematics, University of Waterloo, Canada, 2000–2003

Postdoctoral Research Associate, Department of Chemistry (QTP), University of Florida, 1997–1998

Visiting Assistant Professor, Department of Chemistry, University of Toronto, Canada, 1995–1997

Visiting Assistant Professor, Department of Applied Mathematics, University of Waterloo, Canada, 1994–1995

Postdoctoral Research Associate, Department of Chemistry, University of Arizona, 1992–1993

Adjunct, Institute of Chemistry, University of Wrocław, Poland, 1990–1992

Postdoctoral Fellow, Department of Applied Mathematics, University of Waterloo, Canada, 1988–1991

* Also at: Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824-1322, USA.

Selected Awards and Honors

Elected Fellow of the American Physical Society, 2008
University Distinguished Professor, Michigan State University, 2007
The S.R. Palit Memorial Lecture, Indian Association for the Cultivation of Science, Kolkata, India, 2007
Invitation Fellowship of the Japan Society for the Promotion of Science, 2005
QSCP Promising Scientist Prize of Centre de Mécanique Ondulatoire Appliquée (France) “For Scientific and Human Endeavour and Achievement,” 2004
Elected Corresponding Member of the European Academy of Sciences, Arts, and Humanities (Paris, France), 2003–present
Alfred P. Sloan Research Fellow, 2002-2004
Wiley–International Journal of Quantum Chemistry Young Investigator Award, 2000
The Polish Chemical Society Award for Research (twice), 1992, 1986
The Minister of National Education of Poland Award for Outstanding Doctoral Dissertation, 1989
The President of the University of Wrocław Award for Research (five times), 1991, 1987, 1986, 1985, 1983
The Polish Chemical Society Award for the Best Master of Science Dissertation in Poland in Academic Year 1982/83, 1983
The Polish Academy of Sciences Award for Undergraduate Research in Chemistry (twice), 1982

Publications, Invited Lectures, and Conference Presentations

As of August 13, 2009, 169 scientific publications in peer-reviewed journals and books (79 published or in press after submitting the tenure promotion package; 106 published or in press after joining MSU), including 20 invited book chapters, advanced reviews, and feature articles (14 written after submitting the tenure promotion package; 16 from MSU) and 30 other invited articles (19 written after submitting the tenure promotion package; 22 from MSU), 112 invited lectures (80 given after submitting the tenure promotion package; 98 after joining MSU), including 54 invited talks at major national and international symposia and two named/distinguished lectures, 199 conference presentations (128 given after submitting the tenure promotion package; 155 after joining MSU).

According to the ISI Web of Science, as of August 27, 2009, the scientific articles authored or co-authored by Piotr Piecuch, excluding conference proceedings, have received 4,826 citations (Hirsch’s h-index = 42; 30.16 citations per paper; 1,043 articles excluding self-citations citing Piotr Piecuch’s papers).

Research Interests

Theoretical and computational chemistry and physics, in particular: many-body problem in quantum mechanics; quantum theory of molecular electronic structure; quantum theory of nuclear structure; coupled-cluster theory for finite and extended systems; new *ab initio* methods; new algorithms and computer codes for quantum chemistry; accurate *ab initio* calculations of molecular potential energy surfaces, property functions, and excited states; theoretical reaction dynamics and spectroscopy; reaction mechanisms in organic and bioinorganic chemistry; theory of intermolecular forces, including non-additive interactions between atoms and molecules. *Mathematical methods in chemistry and physics*, in particular: diagrammatic and algebraic methods for many-body systems; the Racah-Wigner algebra; graphical methods of the angular momentum theory; group theory; numerical methods; nonlinear equations; symbolic computations.

Teaching Interests

Development of course curriculum that stresses computer applications in chemistry. Emphasizing precision in formulating and addressing scientific problems. Giving equal weight to analytic reasoning and broadly based education. Using active learning and in-class discussions to encourage students to be creative and think critically. Teaching history of scientific discoveries.

Grant Support

National Science Foundation, PHY-Nuclear Theory, “Nuclear Structure, Nuclear Astrophysics, and Mesoscopic Physics,” co-PI (with B.A. Brown, M. Horoi, and V. Zelevinsky), \$ 540,000, 06/01/08–05/31/11 (awarded).

U.S. Department of Energy, Office of Science, “New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States,” PI, \$ 360,000, 06/01/07–05/31/10 (current).

Japan Society for the Promotion of Science, the JSPS Invitation Fellowship for Research in Japan, awardee, a daily maintenance allowance of 18,000 Japanese yen, domestic research travel allowance of 150,000 Japanese yen, and host’s cooperation allowance of 50,000 Japanese yen (to be used by the host), 10/01/05–11/30/05.

Michigan State University, REF Program, “A High Performance Computing Center for Michigan State University,” co-PI (with L. Kempel, S. Mahanti, F. Jaber, and G. Bao), \$ 3,105,000, 11/11/04–06/30/09 (current).

U.S. Department of Energy, Office of Science, “New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States,” PI, \$ 330,000, 09/01/04–05/31/07.

National Science Foundation, ITR Small Grants, “Development of Parallel Coupled-Cluster Methods,” co-PI (with M.S. Gordon, R.A. Kendall, and M.W. Schmidt), \$499,843 (\$ 166,646 for P. Piecuch), 09/01/03–08/31/06.

The Alfred P. Sloan Research Foundation, \$ 40,000, 09/16/02–09/15/04.

U.S. Department of Energy, Office of Science, “New Coupled-Cluster Methods for Molecular Potential Energy Surfaces,” PI, \$ 340,545, 09/01/01–08/31/04.

National Science Foundation, CHE-Chemical Instrumentation, “Purchase of a High-Performance Parallel Computer,” co-PI (with G.T. Babcock, J.F. Harrison, K.L. Hunt, and J.E. Jackson), \$ 200,000, 08/15/99–07/31/02.

Michigan State University, Intramural Research Grant Program, Science and Engineering Award (New Faculty), “Ab Initio Studies of Photoinduced Charge Transfer in van der Waals Molecules,” PI, \$ 50,000, 05/15/99–09/15/00.

List of Graduate and Undergraduate Research Students, and Postdoctoral Scholars Sponsored

Postdoctoral and visiting scholars (11): Dr. Wei Li, Postdoctoral Associate, October 2007–present (4 papers from MSU); Dr. Marta Włoch, Postdoctoral Associate, November 2003 and January 2004–February 2006, Research Assistant Professor, March 2006–July 2007 (Ph.D., January 2004; 31 publications from MSU, one more with P. Piecuch from MTU; since August 2007, Assistant Professor at Michigan Technological University); Professor Masahiro Ehara (2 publications with PP; currently, Professor at the Institute for Molecular Science, Okazaki, Japan); Dr. Armagan Kinal, NATO-B1/TUBITAK Postdoctoral Fellow, September 2004–March 2005, Postdoctoral Associate, March 2005–August 2006 (Ph.D., June 2004; 6 publications from MSU; since September 2006, Assistant Professor (Associate Docent) at Ege University, Izmir, Turkey); Dr. Karol Kowalski, Postdoctoral Associate, April 1999–June 2004, Research Assistant Professor, June 2004–September 2004 (Ph.D., March 1999; 43 publications from MSU and 2 more with P. Piecuch after leaving MSU; since September 2004, Scientist at

Pacific Northwest National Laboratory); Mr. Tomasz Kuś, Visiting Scholar, January 2004-March 2004 (1 publication from MSU); Professor Stanislaw A. Kucharski, Visiting Professor, January 2004-February 2004 (11 publications with P. Piecuch; Dean of Faculty of Mathematics, Physics, and Chemistry at University of Silesia); Dr. Jiri Pittner, Visiting Scholar, April 2004 (1 publication from MSU; currently, a Research Officer in the J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic); Dr. Rudolf Burcl, Postdoctoral Associate, July 1999-December 2000 (Ph.D., April 1999; 3 publications from MSU; since August 2004, Assistant Professor at Marshall University); Dr. Jesse Edwards, the 1999-00 Affirmative Action Postdoctoral Fellow, September 1999-August 2000 (Ph.D., August 1999, since August 2000, Assistant Professor at Florida Agricultural and Mechanical University, currently, Associate Professor); Dr. Vladimir Špirko, Visiting Associate Professor, November 1998, November and December 1999 (6 publications from MSU; currently, a Principal Research Officer at the Center for Biomolecules and Complex Molecular Systems, Prague, the Czech Republic). *Graduate (Ph.D.) students (9)*: Dr. Ian S.O. Pimienta, former Ph.D. student [Ph.D., December 2003, 7 papers from MSU; Postdoctoral Associate at Iowa State University with Professor M.S. Gordon (2004-2007); currently, Postdoctoral Associate at the University of Utah with Professor J.C. Facelli]; Dr. Peng-Dong Fan, former Ph.D. student [Ph.D., April 2005, 9 papers from MSU; Postdoctoral Associate at University of Florida with Professor S. Hirata (2005-2007); Postdoctoral Associate at Pacific Northwest National Laboratory (2007-2009); currently, Associate Professor at the Theoretical and Computational Laboratory at the Department of Chemistry of Tsinghua University, Beijing, China]; Dr. Ruth C. Jacobsen, former Ph.D. student [co-advised with Professor Katharine C. Hunt; Ph.D., August 2005; Visiting Lecturer at Michigan State University (2005-2007); currently, at Center for Naval Analyses]; Dr. Michael J. McGuire, former Ph.D. student (Ph.D., May 2006, 7 papers from MSU); Dr. Maricris D. Lodrignito, former Ph.D. student (Ph.D., August 2007, 6 papers from MSU; currently, Postdoctoral Associate at Northwestern University with Professor George Schatz); Krzysztof Jedziniak, former graduate student (1 paper from MSU); Jeffrey R. Gour, current Ph.D. student (31 papers from our MSU group, NSF Graduate Research Fellow); Jesse J. Lutz, current Ph.D. student (4 papers from MSU); Janelle Bradley, current Ph.D. student. *Undergraduate Research Students (5)*: Dan Hogan, Spring 1999; Jason Heist, Fall 1999; Elizabeth Kratz, Summer 2000 (the NSF REU Program); Jeffrey R. Gour, Summer 2004 (the NSF REU Program), Fall 2004 and Spring 2005 (currently, an NSF Graduate Research Fellow and a Ph.D. graduate student in our group; cf. above); Bradley S. Elkus, Fall 2006, Fall 2007, Summer 2009-present.

Other Collaborators

Professor Wesley D. Allen, University of Georgia; Professor Rodney J. Bartlett, University of Florida; Professor B. Alex Brown, Michigan State University; Professor Christopher J. Cramer, University of Minnesota; Professor Imre G. Csizmadia, University of Toronto (Canada); Dr. David J. Dean, Oak Ridge National Laboratory; Professor Roger L. DeKock, Calvin College; Professor Masahiro Ehara, Kyoto University (Japan); Professor Karl F. Freed, University of Chicago; Professor Laura Gagliardi, University of Geneva (Switzerland); Professor Mark S. Gordon, Iowa State University and Ames Laboratory; Professor So Hirata, University of Florida; Professor Morten Hjorth-Jensen, University of Oslo (Norway); Dr. Mihai Horoi, Central Michigan University; Professor Katharine C. Hunt, Michigan State University; Professor Stanisław A. Kucharski, University of Silesia (Poland); Dr. Joseph I. Landman, Silicon Graphics, Inc.; Professor Shuhua Li, Nanjing University; Professor Horia Metiu, University of California, Santa Barbara; Dr. Felicja Mrugała, Nicholas Copernicus University (Poland); Professor Debashis Mukherjee, Indian Association for the Cultivation of Science (India); Dr. Monika Musiał, University of Silesia (Poland); Professor Hiroshi Nakatsuji, Kyoto University (Japan); Professor Marcel Nooijen, University of Waterloo (Canada); Dr. Jiri Pittner, Academy of Sciences of the Czech Republic; Professor John C. Polanyi, University

of Toronto (Canada); Dr. Cristina Puzzarini, University of Bologna (Italy); Professor Robert Roth, Technische Universität Darmstadt (Germany); Professor Henry F. Schaefer III, University of Georgia; Dr. Michael W. Schmidt, Iowa State University and Ames Laboratory; Professor C. David Sherrill, Georgia Institute of Technology; Dr. Vladimir Špirko, Academy of Sciences of the Czech Republic; Professor Donald G. Truhlar, University of Minnesota; Professor Antonio J.C. Varandas, University of Coimbra (Portugal); Professor Theresa L. Windus, Iowa State University.

Former Graduate and Postdoctoral Advisors

Professor Henryk Ratajczak, University of Wrocław, Poland, M.S. and Ph.D. advisor
Professor Josef Paldus, University of Waterloo, Canada, postdoctoral advisor
Professor Ludwik Adamowicz, University of Arizona, postdoctoral advisor
Professor John C. Polanyi, University of Toronto, Canada, postdoctoral advisor
Professor Rodney J. Bartlett, University of Florida, postdoctoral advisor.

Editorial Boards

International Journal of Quantum Chemistry (published by Wiley), Member of the Editorial Board (January 2005–present).

Journal of Computational Methods in Science and Engineering (published by IOS Press), Member of the Editorial Board (January 2005–present).

The Open Chemical Physics Journal (published by Bentham Science Publishers), Member of the Editorial Board (Vol. 1, 2007–present).

Open Chemical Physics Reviews (published by Bentham Science Publishers), Member of the Editorial Board (Vol. 1, 2007–present).

Progress in Theoretical Chemistry and Physics (book series published by Springer), Member of the Editorial Board (Vol. 16, 2007 – present).

Interdisciplinary Sciences: Computational Life Sciences (the official publication of the International Association of Scientists in the Interdisciplinary Areas, IASIA, in partnership with Springer), Member of the Editorial Board (Vol. 1, 2008–present).

Research Letters in Physical Chemistry (published by Hindawi Publishing Corporation), Member of the Editorial Board (July 2009–present).

Meetings Organized and Membership in Organizing Committees and International Advisory Boards

Organizer of the Workshop “High-Performance Computer Center at Michigan State University,” Michigan State University, East Lansing, Michigan, U.S.A., November 2, 2003 (Chair of the Organizing Committee).

Organizer of the 36th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 17-19, 2004 (Chair of the Organizing Committee).

Member of the Local Organizing Committee for the Workshop “Nuclei and Mesoscopic Physics,” Michigan State University, East Lansing, Michigan, U.S.A., October 23-26, 2004.

Co-organizer of the 2nd Workshop on Nuclei and Mesoscopic Physics, WNMP07, Michigan State University, East Lansing, Michigan, U.S.A., October 20-22, 2007.

Chair of the Local Organizing Committee for the Thirteenth International Workshop Quantum Systems in Chemistry and Physics (QSCP-XIII), Lansing, Michigan, U.S.A., July 6-12, 2008.

Member of the Local Organizing Committee for the Sixth Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver, British Columbia, Canada, July 19-24, 2008.

Organizer of the Symposium on Coupled-Cluster Theory (CCT) during the Sixth Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver, British

Columbia, Canada, July 19-24, 2008 (July 19-20, 2008).
Member of the International Scientific Committee for a conference series Quantum Systems in Chemistry and Physics (QSCP).
Member of the International Advisory Committee for a conference series “Molecular Spectroscopy.”
Member of the International Scientific Committee for the Sixth Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver, British Columbia, Canada, July 19-24, 2008.

Other Examples of National and International Professional Service

Session Chair, The symposium “Electronic Structure Theory: From Methods to Molecules and Materials,” 100th Annual Meeting of the American Physical Society, Atlanta, Georgia, U.S.A., March 21-26, 1999.
Session Chair, “Vth International Conference on Molecular Spectroscopy,” Łądek-Zdrój, Poland, September 26-30, 1999.
Session Chair, International Symposium on Frontiers in Molecular Science 2002, Qingdao, China, July 15-18, 2002.
Special Session Chair, Ninth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-IX, Les Houches, France, September 25-30, 2004.
Session Chair, the symposium “Theoretical Determination of Energy Landscapes: Methodology and Applications,” 230th American Chemical Society National Meeting, Washington, DC, U.S.A., August 28-September 1, 2005.
Session Chair, Tenth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-X, Carthage, Tunisia, September 1-7, 2005.
Session Chair, 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.
Session Chair, Twelfth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XII, London, U.K., August 30 - September 5, 2007.
Session Chair, 2nd Workshop on Nuclei and Mesoscopic Physics, WNMP07, Michigan State University, East Lansing, Michigan, U.S.A., October 20-22, 2007.
Session Chair, Thirteenth International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XIII, Lansing, Michigan, U.S.A., July 6-12, 2008.
Session Chair, Sixth Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver, British Columbia, Canada, July 19-24, 2008.
Session Chair, the WE-Heraeus-Seminar “Ab-Initio Nuclear Structure - Where do we stand?”, Bad Honnef, Germany, July 28-30, 2008.
Session Chair, The International Conference on the Theory and Applications of Computational Chemistry in 2008 (TACC 2008), Shanghai, China, September 23-27, 2008.
Session Chair, The symposium “Advances in Electronic Structure Theory and First Principles Dynamics,” 237th American Chemical Society National Meeting, Salt Lake City, Utah, U.S.A., March 22-26, 2009.
Session Chair, International Workshop “Linking Nuclei, Molecules, and Condensed Matter: Computational Quantum Many-Body Approaches,” European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Trento, Italy, July 6-10, 2009.
Session Chair, The symposium “New Developments in Strongly Correlated Electrons,” 238th American Chemical Society National Meeting, Washington, DC, U.S.A., August 16-20, 2009.
Session Chair, The 50th Sanibel Symposium, St. Simons Island, Georgia, U.S.A., February 24-March 2, 2010.
Referee for *Science*, *Physical Review Letters*, *Physical Review A*, *Physical Review B*, *Chemical Physics Letters*, *Journal of Chemical Physics*, *Molecular Physics*, *Computer Physics Communications*, *European Physics Journal A*, *European Physics Journal D*, *Theoretica Chimica Acta*, *Theoretical Chemistry Accounts*, *International Journal of Quantum Chemistry*, *Journal of Chemical Theory and Computation*, *Journal of Molecular Structure (THEOCHEM)*, *Journal of Physical Chemistry*, *Journal of the American Chemical Society*, *Canadian Journal*

of Chemistry, Collection of Czechoslovak Chemical Communications, Spectroscopy Letters, International Journal of Molecular Sciences, Progress of Theoretical Chemistry and Physics, Cambridge University Press, and Oxford University Press.

Reviewer of proposals submitted to the *National Science Foundation*, the *US Department of Energy*, the *Petroleum Research Fund*, the *Air Force Office of Scientific Research*, the *United States Civilian Research and Development Foundation for the Independent States of the Former Soviet Union*, the *Alfred P. Sloan Foundation*, the *Research Corporation*, the *Computational Center for Molecular Structure and Interactions* sponsored by the *National Science Foundation's CREST Program*, the *Fonds voor Wetenschappelijk Onderzoek – Vlaanderen* (Belgium), the *Engineering and Physical Sciences Research Council* (U.K.), and the *Grant Agency at the Academy of Sciences of the Czech Republic*. I served as a member of the *US Department of Energy, Theory, Modeling, and Simulation in Nanoscience Review Panel* in 2003.

Service to the Department, College, and the University (MSU)

Member of the University Appeals Board, 2001–2007
Member of the Chemical Physics Committee, 2000–present
Member of the Center for Biological Modeling, 2000–2004
Member of the Quantitative Biology and Modeling Initiative, 2004–present
Chair of the Chemistry Department Computer Committee, 2000–2003
Member of the Chemistry Department Computer Committee, 1998–present
Member of the Chemistry Department Graduate Admissions Committee, 2003/2004
Member of the Chemistry Department Graduate Advising Committee, 2004/2005
Member of the High Performance Computing Center Advisory Committee, 2004–present
Member of the Mesoscopic Theory Center, 2006–present
Member of Visioning Committee for Cyber Enabled Discovery, 2008
Member of the Leadership Team for Institute for Cyber Enabled Research, 2008
Member of the Chemistry Department Reappointment and Promotion Committee, 2008/2009

Other Examples of Synergistic Activities

Co-author of the electronic structure package GAMESS (Coupled-Cluster codes; registered user base over 20,000 (2006)); contributor of potential energy surfaces to the on-line library POTLIB.

Press Releases and Popular Feature Articles on Our Research (Selected Examples)

“MSU prof provides insight on atomic nuclei,” by Matthew Miller, *Lansing State Journal*, April 23, 2007,

“Coupled-clusters point to faster computation,” *CERN Courier*, Vol. 47, No. 4, May 1, 2007,

“Physicists wipe away complexity for a clearer view of heavy nuclei,” *AAAS EurekAlert*, March 14, 2007,

“Beyond the nuclear shell model,” *Physics Today*, November 2007, and dozens of other articles.

The article C.J. Cramer, M. Włoch, P. Piecuch, C. Puzzarini, and L. Gagliardi, *J. Phys. Chem. A* **110**, 1991-2004 (2006) has been recognized as one of the “Most-Cited Articles Published in 2006” in *The Journal of Physical Chemistry A* (see http://pubs.acs.org/journals/jpcafh/promo/most/most_cited/2006.html).

The Air Force Office of Scientific Research STTR 09.B solicitation calling for proposals on Coupled Cluster Methods for Multi-Reference Applications (AF09-BT40; see <http://www.dodsbir.net/solicitation/sttr09B/af09B.htm>) used our advances in areas of renormalized and equation-of-motion coupled-cluster methods as a motivation for a call for new proposals. Two of the three papers cited in this solicitation [*Adv. Quantum Chem.* **34**, 295 (1999) and *Int. Rev. Phys. Chem.* **21**, 527 (2002)] are by P. Piecuch and co-workers.

Professional Societies

European Academy of Sciences, Arts, and Humanities (Paris, France; Elected Member), American Physical Society (Elected Fellow), American Chemical Society (member), American Association for the Advancement of Science (member), International Society for Theoretical Chemical Physics (member), World Association of Theoretical and Computational Chemists (life member), Polish Chemical Society (member)

Other Societies

International Society of Friends of Wrocław University (elected; Honorary President: Professor W.J. Orville-Thomas, President: Professor A. Müller)