

CURRICULUM VITAE

Dr. Piotr Piecuch, University Distinguished Professor, MSU Research Foundation Professor
Department of Chemistry, Michigan State University
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Education

Ph.D., 1988, University of Wrocław, Poland (with Distinction)
M.S., 1983, University of Wrocław, Poland (with Distinction)

Professional Experience

Michigan State University

MSU Research Foundation Professor, Department of Chemistry, Michigan State University, 2020–present
University Distinguished Professor, Department of Chemistry, Michigan State University, 2007–present
Adjunct Professor, Department of Physics and Astronomy, Michigan State University, 2004–2010, 2014–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

Clark Way Harrison Distinguished Visiting Professor, Department of Chemistry, Washington University in St. Louis, 2016 (5 months)
Invited Professor and Scientist (equivalent to Visiting Professor), Institute for Molecular Science, National Institutes of Natural Sciences, Okazaki, Japan, 2012/2013 (3 months)
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
Assistant Professor (tenure track; in Polish, “Adiunkt”), Institute of Chemistry (presently, Faculty of Chemistry), University of Wrocław, Poland, 1990–1992 (resigned)

* Also, Adjunct Professor at Department of Physics and Astronomy, Michigan State University.

Postdoctoral Fellow, Department of Applied Mathematics, University of Waterloo, Canada, 1988–1991
Senior Assistant (in Polish, “Starszy Asystent”), Institute of Chemistry (presently, Faculty of Chemistry), University of Wrocław, Poland, 1985–1990
Assistant (in Polish, “Asystent”), Institute of Chemistry (presently, Faculty of Chemistry), University of Wrocław, Poland, 1984–1985
Junior Assistant (in Polish, “Młodszy Asystent”), Institute of Chemistry (presently, Faculty of Chemistry), University of Wrocław, Poland, 1983–1984

Awards and Honors

MSU Research Foundation Professor, Michigan State University, 2020
The Xingda Lectureship, College of Chemistry and Molecular Engineering, Peking University, Beijing, China, 2019
Elected Member of the International Academy of Quantum Molecular Science, 2018
The Lawrence J. Schaad Lectureship in Theoretical Chemistry, Vanderbilt University, 2017
Fellow of the Royal Society of Chemistry, 2016
Clark Way Harrison Distinguished Visiting Professor, Washington University in St. Louis, 2016
Distinguished Fellow of the Kosciuszko Foundation Collegium of Eminent Scientists, 2015
Outstanding Reviewer for *Chemical Physics Letters* (Elsevier), 2014
Invited Professor and Scientist (Visiting Professor) at the Institute for Molecular Science, Okazaki, Japan, 2012/2013
Fellow of the American Association for the Advancement of Science, 2011
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
Professor Catedrático Visitante (Visiting Professor) at the University of Coimbra, Portugal, 2006
Invitation Fellowship of the Japan Society for the Promotion of Science and Visiting Professorship at Kyoto University, 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
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 Papers (February 20th, 2024)

- 235 publications in peer-reviewed journals and books (145 after submitting the tenure promotion package; 172 after joining MSU), including 23 invited book chapters, advanced reviews, and feature articles (17 written after submitting the tenure promotion package; 19 from MSU) and 54 other invited articles (43 written after submitting the tenure promotion package; 46 from MSU).

- 6 edited books and 2 edited special journal issues.
- 296 invited lectures (264 given after submitting the tenure promotion package; 282 after joining MSU), including 155 invited talks at national and international symposia and three named lectures.
- 373 conference presentations (302 given after submitting the tenure promotion package; 330 after joining MSU).
- Citations: 14,849 (Web of Science; MSU subscription), 16,714 (Google Scholar).
- Citations per paper: 63.46; articles excluding self-citations citing Piotr Piecuch's papers: 4,958; 1 paper cited 600+ times, 1 paper cited 500+ times, 4 papers cited 400+ times, 6 papers cited 300+ times, 17 papers cited 200+ times, and 41 papers cited 100+ times (Web of Science; MSU subscription). Google Scholar reported 1 paper cited 800+ times, 1 paper cited 700+ times, 1 paper cited 600+ times, 2 papers cited 500+ times, 4 papers cited 400+ times, 8 papers cited 300+ times, 20 papers cited 200+ times, and 51 papers cited 100+ times.
- *h*-index: 66 (Web of Science), 72 (Google Scholar).

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; local correlation and fragmentation electronic structure approaches for large molecular systems; 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; catalysis; structural and electronic properties of transition metal nanoparticles; photochemistry; 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

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, \$474,999, 12/01/21–06/30/25 (current).

National Science Foundation, CHE–Chemical Theory, Models and Computational Methods, "High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," PI, \$420,000, 07/01/18–06/30/22.

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, \$493,061,

12/01/18–11/30/21.

Defense Advanced Research Projects Agency, “Super-Photoreagents as a Gateway to Precision Chemistry,” co-PI (with M. Dantus, G.J. Blanchard, B. Borhan, and J.E. Jackson), \$799,403
12/01/19–11/30/20.

National Science Foundation, OAC–Office of Advanced Cyberinfrastructure, via Virginia Polytechnic Institute and State University, “S2I2: Impl: The Molecular Sciences Software Institute,” PI: T.D. Crawford, co-PIs: T. Head-Gordon, V. Pande, T. Windus, and S. Jha, Michigan State University subaward PI: P. Piecuch, Phase I and Phase II MolSSI Software Fellowships awarded to a Ph.D. student in the Piecuch group, J.E. Deustua, \$90,739, 07/01/18–06/30/20.

Michigan State University Foundation, Strategic Partnership Grants Program, “De Novo Computational Methods for Simulating Energy Materials,” co-PI (with Y. Qi, H.M. Aktulga, and W. Lai), \$399,299 (25 % for P. Piecuch), 07/01/16–06/30/19.

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, \$482,950, 12/01/15–11/30/18.

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, 06/01/13–11/30/15.

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, \$518,000, 06/01/10–05/31/13.

The Air Force Office of Scientific Research (AFOSR) through Spectral Sciences, Inc., the Small Business Technology Transfer (STTR) Program, “Innovative Approaches to Scalable and Multi-reference Coupled Cluster Methods,” co-PI (with M. Braunstein and M.S. Gordon), \$100,000 (\$30,000 for P. Piecuch), 05/03/10–02/02/11.

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; unused by P. Piecuch due to budget reduction).

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.

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.

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 (16): Martyna Osada, Visiting Scholar, November 2022 (on leave from the Faculty of Physics, University of Warsaw, Poland); Dr. Suhita Basu Mallick, Postdoctoral Research Associate, September 2021 – April 2023 (Ph.D., August 2021); Dr. Jun Shen, Postdoctoral Research Associate, December 2010 – November 2013, Research Assistant Professor (fixed-term), December 2013 – November 2014, Postdoctoral Research Associate, December 2014 – May 2016, Senior Research Associate, May 2016 – present (Ph.D., October 2008; 31 papers from work with P. Piecuch at MSU); Dr. Wei Li, Postdoctoral Associate, October 2007 – May 2010, Research Assistant Professor, June–December 2010 (Ph.D., August 2007; 10 papers from work with P. Piecuch at MSU; currently, Associate Professor in School of Chemistry and Chemical Engineering at Nanjing University, China); Dr. Jeffrey R. Gour, Postdoctoral Associate, May–July 2010 [Ph.D., April 2010, 37 papers from work with P. Piecuch at MSU; Postdoctoral Associate at Stanford University with Professor Todd J. Martinez (2010-2011); Technical Support Analyst at Epic (2011-2014); IT Analyst at Alliant Energy (2014-2015); Software Design Engineer at Sonic Foundry (2015-2017); Software Development Engineer at Amazon (2017-2018); Software Development Lead at Sonic Foundry (2018-2020); currently (2020-), Senior Software Engineer at Microsoft]; 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 work with P. Piecuch at MSU plus 8 more in collaboration with P. Piecuch after leaving MSU; Assistant Professor at Michigan Technological University (2007-2011); Assistant Professor at Oakland University (2011-2019); Student Teacher at Seaholm High School, Birmingham, Michigan (2019); Chemistry Teacher at Stoney Creek High School, Rochester, Michigan (2019); Chemistry Instructor, Macomb Community College, Warren, Michigan (2020); Academic Specialist and Chemistry Instructor in the Lyman Briggs College at Michigan State University (2020-2021); currently (2022-), Chemistry Teacher at St. Mary’s Preparatory, Orchard Lake, Michigan]; Professor Jozef Noga, Visiting Professor, May 2010 (Professor at Comenius University and Slovak Academy of Sciences, Bratislava, Slovakia); Professor Masahiro Ehara, Visiting Professor, October 2007 – November 2007, March 2011 (5 publications with P. Piecuch; 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 work with P. Piecuch at MSU; since January 2007 at Ege University, Izmir, Turkey: Assistant Professor (2007-2011), Associate Professor (2011-2018), currently (2018-), Full Professor]; Dr. Karol Kowalski, Postdoctoral Associate, April 1999 – June 2004, Research Assistant Professor, June 2004 – September 2004 [Ph.D., March 1999; 44 publications from work with P. Piecuch at MSU plus 2 more in collaboration with P. Piecuch after leaving MSU; since September 2004 at the Pacific Northwest National Laboratory: Research Scientist Level III (2004-2007), Research Scientist Level IV (2007-2010), Research Scientist Level V (Chief Scientist, 2010-2019), currently (2019-), Laboratory Fellow]; Dr. Tomasz Kuś, Visiting Scholar, January 2004 – March 2004 [on leave from the Institute of Chemistry at the University of Silesia, Poland; 1 publication from work with P. Piecuch at MSU; currently (2016-), Principal Software Engineer at DNV, Gdynia Poland]; Professor Stanisław A. Kucharski, Visiting Professor, January 2004 – February 2004 (11 publications with P. Piecuch; Professor and former Vice President for Finance and Development and former Director of the Institute of Chemistry at the University of Silesia, Poland); Dr. Jiri Pittner, Visiting Scholar, April 2004 (1 publication from MSU; currently, Head of the Department of Theoretical Chemistry at 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 work with P. Piecuch at MSU; Assistant Professor at Marshall University (2004-2011); currently, physician (MD) at Cheyenne Regional Medical Center]; Dr. Jesse Edwards, the 1999-00 Affirmative Action Postdoctoral Fellow, September 1999 – August 2000 (Ph.D., Au-

gust 1999; since August 2000 on the faculty of Florida Agricultural and Mechanical University, currently Full Professor); Dr. Vladimir Špirko, Visiting Associate Professor, November 1998, November and December 1999 (11 publications with P. Piecuch, including 6 publications from MSU; currently, Emeritus at the Institute of Organic Chemistry and Biochemistry of the Academy of Sciences of the Czech Republic). *Graduate (Ph.D.) students (20)*: Dr. Ian S.O. Pimienta, former Ph.D. student [1999-2003, Ph.D., December 2003, 7 papers from work with P. Piecuch at MSU; Postdoctoral Associate at Iowa State University with Professor M.S. Gordon (2004-2007) and at the University of Utah with Professor J.C. Facelli (2007-2010); Assistant Professor at Troy University (2010-2016); Postdoctoral Associate at Auburn University with Professor K. Patkowski (2017-2019); currently (2019-), Assistant Professor at the University of Pikeville]; Dr. Peng-Dong Fan, former Ph.D. student [2001-2005, Ph.D., April 2005, 9 papers from work with P. Piecuch at MSU; Postdoctoral Associate at the University of Florida with Professor S. Hirata (2005-2007); Postdoctoral Associate at the Pacific Northwest National Laboratory (2007-2009)]; Dr. Ruth L. Jacobsen, former Ph.D. student [1999-2005, co-advised with Professor Katharine C. Hunt, Ph.D., August 2005; Visiting Lecturer at Michigan State University (2005-2007); Research Analyst at Center for Naval Analyses (2007-2009); NIST-ARRA (American Reinvestment and Recovery Act) Senior Fellowship (2010-2011); Visiting Senior Research Scientist at NIST (2011-2015); Hazardous Materials Program Manager at Marine Corps Base Quantico (2015-2018)]; Dr. Michael J. McGuire, former Ph.D. student (2000-2006, Ph.D., May 2006, 7 papers from work with P. Piecuch at MSU); Dr. Maricris Lodrignito Mayes, former Ph.D. student [2002-2007, Ph.D., August 2007, 6 papers from work with P. Piecuch at MSU; Postdoctoral Associate at Northwestern University with Professor G.C. Schatz (2007-2011); Postdoctoral Appointee at the Leadership Computing Facility at Argonne National Laboratory (with Dr. G. Fletcher and Professor M.S. Gordon, 2011-2013); since 2014, on the faculty of the University of Massachusetts Dartmouth, currently (2020-), Associate Professor]; Dr. Jeffrey R. Gour, former Ph.D. student [2005-2010, Ph.D., April 2010, 37 papers from work with P. Piecuch at MSU; NSF Graduate Research Fellow (2005-2009); Postdoctoral Associate at Stanford University with Professor T.J. Martinez (2010-2011); Technical Support Analyst at Epic (2011-2014); IT Analyst at Alliant Energy (2014-2015); Software Design Engineer at Sonic Foundry (2015-2017); Software Development Engineer at Amazon (2017-2018); Software Development Lead at Sonic Foundry (2018-2020); currently (2020-), Senior Software Engineer at Microsoft]; Dr. Jesse J. Lutz, former Ph.D. student [2006-2011, Ph.D., August 2011, 13 papers from work with P. Piecuch at MSU; Postdoctoral Associate at Durham University, U.K., with Professor J.M. Hutson (2011-2014); Visiting Scientist at the University of Florida with Professor R.J. Bartlett (2015-2016); Research Assistant Professor at the Air Force Institute of Technology with Professor L.W. Burggraf (2015-2019); currently (2019-), Senior Member of Technical Staff in the Center for Computing Research at the Sandia National Laboratories]; Krzysztof Jedziniak, former graduate student (2001-2002, 1 paper from work with P. Piecuch at MSU; last known appointments, Investment Director, UK Trade and Investment, and Consultant in Warsaw-based Bureau of A.T. Kearney); Dr. Janelle A. Bradley, former graduate student (2008-2010); Dr. Jared A. Hansen, former Ph.D. student [2010-2015, Ph.D., September 2015, 10 papers from work with P. Piecuch at MSU; Postdoctoral Associate at the University of Michigan in Ann Arbor with Professor P.M. Zimmerman (2015-2016)]; Dr. Nicholas P. Bauman, former Ph.D. student [2011-2016, Ph.D., November 2016, 7 papers from work with P. Piecuch at MSU; Postdoctoral Associate at the University of Florida with Professor R.J. Bartlett (2017); Postdoctoral Associate at the Pacific Northwest National Laboratory with Dr. Karol Kowalski (2018-2022); currently (2022-), Research Scientist Level III at the Pacific Northwest National Laboratory]; Dr. Adeayo O. Ajala, former Ph.D. student [2012-2017, Ph.D., December 2017, 3 papers from work with P. Piecuch at MSU; Postdoctoral Associate at the University of California San Diego with Professor Francesco Paesani (2018-2019); currently (2019-), Process Chemist at TOK America]; Dr. Jorge Emiliano Deustua, former Ph.D. student [2014-2020, Ph.D., May 2020, 10 papers from work with P. Piecuch at MSU; Phase I and Phase II MolSSI Software Fellow (2018-

2020); Postdoctoral Associate at California Institute of Technology with Professor Thomas F. Miller III (2020-2022); Software Engineer at Emptor (2022-2023); currently (2023-), COO and Co-founder at Examol]; Dr. Ilias Magoulas, former Ph.D. student [2015-2021; Ph.D., March 2021, 14 papers from work with P. Piecuch at MSU; currently (2021-), Postdoctoral Associate at Emory University with Professor Francesco Evangelista]; Dr. Stephen H. Yuwono, former Ph.D. student [2017-2022; Ph.D., May 2022, 12 papers from work with P. Piecuch at MSU; currently (2022-), Postdoctoral Associate at Florida State University with Professor A. Eugene DePrince III]; Arnab Chakraborty, current Ph.D. student (2018-present; 3 papers from work with P. Piecuch at MSU); Karthik Gururangan, current Ph.D. student (2019-present; 4 papers from work with P. Piecuch at MSU); Tiange Deng, current Ph.D. student (2021-present); Swati Snigdha Priyadarsini, current Ph.D. student (2021-present; 2 papers from work with P. Piecuch at MSU); Agnibha Hanra, current Ph.D. student (2022-present). *Undergraduate Research Students (6)*: 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 (an NSF Graduate Research Fellow and a former Ph.D. graduate student and postdoc in our group; cf. above); Bradley S. Elkus, Fall 2006, Fall 2007, Summer 2009, Fall 2009; Jonathon Clapham, Fall 2011.

Other Former and Current Senior Collaborators

Professor Ludwik Adamowicz, University of Arizona; Professor Igor Aharonovich, University of Technology Sydney (Australia); Professor H. Metin Aktulga, Michigan State University; Professor Ali Alavi, Max-Planck-Institut für Festkörperforschung (Germany) and University of Cambridge (United Kingdom); Professor Wesley D. Allen, University of Georgia; Professor Rodney J. Bartlett, University of Florida; Professor Gary J. Blanchard, Michigan State University; Dr. Valérie Blanchet, Université de Bordeaux (France); Dr. Ota Bludský, Academy of Sciences of the Czech Republic; Professor Babak Borhan, Michigan State University; Professor Weston Thatcher Borden, University of North Texas; Dr. Carlo Bradac, University of Technology Sydney (Australia); Professor B. Alex Brown, Michigan State University; Professor Grzegorz Chałasiński, University of Warsaw (Poland); Professor Garnet Kin-Lic Chan, California Institute of Technology; Professor Rajat K. Chaudhuri, Indian Institute of Astrophysics; Professor Cheol Ho Choi, Kyungpook National University (South Korea); Professor Jiří Čížek, University of Waterloo (Canada); Professor Christopher J. Cramer, University of Minnesota; Professor Imre G. Csizmadia, University of Toronto (Canada); Professor Marcos Dantus, Michigan State University; Dr. David J. Dean, Oak Ridge National Laboratory; Professor Roger L. DeKock, Calvin College; Professor Masahiro Ehara, Institute for Molecular Science, Okazaki (Japan); Professor Janus J. Eriksen, Technical University of Denmark (Denmark); Professor Michael Filatov, Kyungpook National University (South Korea); Professor Michael J. Ford, University of Technology Sydney (Australia); Professor Karl F. Freed, University of Chicago; Professor Laura Gagliardi, University of Chicago; Professor Jürgen Gauss, Johannes Gutenberg-Universität Mainz (Germany); Professor Yingbin Ge, Central Washington University; Professor Mark S. Gordon, Iowa State University and Ames Laboratory; Professor William H. Green, Massachusetts Institute of Technology; Professor Martin Head-Gordon, University of California, Berkeley; Professor So Hirata, University of Illinois at Urbana-Champaign; Professor Morten Hjorth-Jensen, University of Oslo (Norway; currently, also, Michigan State University); Professor Mark R. Hoffmann, University of North Dakota; Professor Mihai Horoi, Central Michigan University; Professor James E. Jackson, Michigan State University; Professor Karol Jankowski, Nicholas Copernicus University (Poland); Professor Maria Jaworska, University of Silesia (Poland); Professor Bogumił Jeziorski, University of Warsaw (Poland); Professor Taiha Joo, Pohang University of Science and Technology (POSTECH; South Korea); Dr. Mehran Kianinia, University of Technology Sydney (Australia); Professor Paweł M. Kozłowski, University of Louisville; Professor Stanisław A. Kucharski, University of Silesia (Poland); Dr. Joseph I. Landman, Scalable Informatics; Professor Zdzisław Latajka, University of Wrocław (Poland); Professor Benjamin G.

Levine, Stony Brook University; Professor Shuhua Li, Nanjing University (China); Professor Wenjian Liu, Shandong University (China); 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); Professor Monika Musiał, University of Silesia (Poland); Professor Hiroshi Nakatsuji, Kyoto University (Japan); Dr. Petr Navrátil, TRIUMF (Canada); Professor Marcel Nooijen, University of Waterloo (Canada); Professor William J. Orville-Thomas, University of Salford (United Kingdom); Professor Sourav Pal, Indian Institute of Science Education and Research, Kolkata (India); Professor Josef Paldus, University of Waterloo (Canada); Professor Thomas F. Papenbrock, University of Tennessee; Professor Katarzyna Pernal, Łódź University of Technology (Poland); Dr. Jiri Pittner, Academy of Sciences of the Czech Republic; Professor John C. Polanyi, University of Toronto (Canada); Professor Cristina Puzzarini, University of Bologna (Italy); Professor Yue Qi, Brown University; Professor Chintamani N.R. Rao, Jawaharlal Nehru Centre for Advanced Scientific Research (India); Professor Henryk Ratajczak, University of Wrocław (Poland); Professor Jeffrey R. Reimers, University of Technology Sydney (Australia) and Shanghai University (China); Professor Robert Roth, Technische Universität Darmstadt (Germany); Professor Pascale Roubin, Université de Provence-CNRS (France); Professor Henry F. Schaefer III, University of Georgia; Dr. Michael W. Schmidt, Iowa State University and Ames Laboratory; Professor Sandeep Sharma, University of Colorado at Boulder; Professor C. David Sherrill, Georgia Institute of Technology; Professor Pedro J. Silva, Universidade Fernando Pessoa (Portugal); Dr. Vladimír Špirko, Academy of Sciences of the Czech Republic; Professor Péter Surján, Eötvös University (Hungary); Professor Malgorzata M. Szczeniak, Oakland University; Professor Seiichiro L. Ten-no, Kobe University (Japan); Professor Donald G. Truhlar, University of Minnesota; Professor Cyrus J. Umrigar, Cornell University; Professor Adri C.T. van Duin, Pennsylvania State University; Professor Antonio J.C. Varandas, University of Coimbra (Portugal); Professor Tomasz A. Wesolowski, University of Geneva (Switzerland); Professor K. Birgitta Whaley, University of California, Berkeley; Professor Angela K. Wilson, Michigan State University; 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 Activities

Guest Co-editor of the Special Issue of the *International Journal of Quantum Chemistry* (Wiley) dedicated to the Proceedings from the Eleventh European Workshop on Quantum Systems in Chemistry and Physics (St. Petersburg, Russia, August 20-25, 2006), *Int. J. Quantum Chem.*, Volume 107, Issue 14 (2007).

Co-editor of Volume 18 of *Progress in Theoretical Chemistry and Physics* (book series published by Springer), published in 2008, entitled “Frontiers in Quantum Systems in Chemistry and Physics,” and dedicated to the Proceedings from the Twelfth European Workshop on Quantum Systems in Chemistry and Physics (London, U.K., August 30 - September 5, 2007).
Co-editor of Volume 995 of AIP Conference Proceedings, published in 2008, entitled *Nuclei and Mesoscopic Physics, Workshop on Nuclei and Mesoscopic Physics, WNMP 2007*.

Co-editor of Volume 19 of *Progress in Theoretical Chemistry and Physics* (book series published by Springer), published in 2009, entitled “Advances in the Theory of Atomic and Molecular Systems: Conceptual and Computational Advances in Quantum Chemistry,” and

dedicated to the Proceedings from the Thirteenth International Workshop on Quantum Systems in Chemistry and Physics (Lansing, Michigan, U.S.A., July 6-12, 2008).

Co-editor of Volume 20 of *Progress in Theoretical Chemistry and Physics* (book series published by Springer), published in 2009, entitled “Advances in the Theory of Atomic and Molecular Systems: Dynamics, Spectroscopy, Clusters, and Nanostructures,” and dedicated to the Proceedings from the Thirteenth International Workshop on Quantum Systems in Chemistry and Physics (Lansing, Michigan, U.S.A., July 6-12, 2008).

Guest Co-editor of the Special Issue of the *International Journal of Quantum Chemistry* (Wiley) dedicated to the Proceedings from the Fourteenth European Workshop on Quantum Systems in Chemistry and Physics (San Lorenzo de El Escorial, Madrid, Spain, September 13-19, 2009), *Int. J. Quantum Chem.*, Volume 111, Issue 2 (2011).

Co-editor of Volume 22 of *Progress in Theoretical Chemistry and Physics* (book series published by Springer), published in 2012, entitled “Advances in the Theory of Quantum Systems in Chemistry and Physics,” and dedicated to the Proceedings from the Fifteenth International Workshop on Quantum Systems in Chemistry and Physics (Cambridge, U.K., August 31 - September 5, 2010).

Co-editor of Volume 26 of *Progress in Theoretical Chemistry and Physics* (book series published by Springer), published in 2012, entitled “Quantum Systems in Chemistry and Physics: Progress in Methods and Applications,” dedicated to the Proceedings from the Sixteenth International Workshop on Quantum Systems in Chemistry and Physics (Kanazawa, Japan, September 11-17, 2011).

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).

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).

Handbook of Research on Computational and Systems Biology: Interdisciplinary Applications (published by IGI Global, 2010).

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; 2006–2013), including QSCP-XI, St. Petersburg, Russia, August 20-25, 2006, QSCP-XII, London, U.K., August 30 - September 5, 2007, QSCP-XIII, Lansing, Michigan, U.S.A., July 6-12, 2008, QSCP-XIV, San Lorenzo de El Escorial, Madrid, Spain, September 13-19, 2009, QSCP-XV, Cambridge, U.K., August 31 - September 5, 2010, QSCP-XVI, Kanazawa, Japan, September 11-17, 2011, QSCP-XVII, Turku, Finland, August 19-25, 2012, QSCP-XVIII, Paraty (Rio de Janeiro), Brazil, December 1-7, 2013.

Member of the International Advisory Committee for a conference series “Molecular Spectroscopy” (IXth edition; Wrocław – Łądek-Zdrój, Poland, September 12-16, 2007).

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.

Member of the International Scientific Committee for the Seventh Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII), Tokyo, Japan, September 2-8, 2011.

Member of the International Advisory Board for the Eighth Congress of the International Society for Theoretical Chemical Physics (ISTCP-VIII), Budapest, Hungary, August 25-31, 2013.

Co-organizer of the symposium “Recent Progress in Molecular Theory for Excited-State Electronic Structure and Dynamics” at the 2015 International Chemical Congress of Pacific Basin Societies (Pacifichem 2015), Honolulu, Hawaii, U.S.A., December 15-20, 2015.

Co-organizer of the Symposium on Electronic Structure Theory (entitled “Advances in Electron Correlation: From Strongly Correlated to Large Systems”) during the Ninth Congress of the International Society for Theoretical Chemical Physics (ISTCP-IX), Grand Forks, North Dakota, U.S.A., July 17-22, 2016.

Co-organizer of the 49th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 1-3, 2017 (Member of the Organizing Committee).

Member of the International Scientific Committee for the conference “Quantum International Frontiers 2018,” Changsha, Hunan Province, China, October 17-21, 2018.

Member of the International Scientific Committee for the Utah Workshop on Quantum Methods in Molecular and Solid-State Theory, Park City, Utah, U.S.A., September 22-27, 2019.

Member of the International Scientific Committee for the conference “Quantum International Frontiers 2019,” Shanghai, China, November 18-22, 2019.

Co-organizer of the Symposium “Advances in Electronic Structure Theory: A Symposium in Honour of Joe Paldus” during the 107th Canadian Chemistry Conference and Exhibition (CSC 2024), Winnipeg, Manitoba, Canada, June 2-6, 2024.

Co-organizer of the Symposium on Wave Function Theory for Electronic Structure during the Eleventh Congress of the International Society for Theoretical Chemical Physics (ISTCP-XI), Qingdao, China, October 13-18, 2024.

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, Fourteenth International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XIV, San Lorenzo de El Escorial, Madrid, Spain, September 13-19, 2009.
Session Chair, An International Symposium “Recent Advances in Many Electron Theories,” Shankarpur, West Bengal, India, January 5-7, 2010.
Session Chair, 31st Annual Combustion Research Meeting, Airlie Conference Center, Warrenton, Virginia, U.S.A., June 1-4, 2010.
Session Chair, Fifteenth International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XV, Magdalene College, Cambridge University, Cambridge, U.K., August 31 - September 5, 2010.
Session Chair, The symposium “Fragment and Local Orbital Methods in Electronic Structure Theory,” 241st American Chemical Society National Meeting, Anaheim, California, U.S.A., March 27-31, 2011.
Session Chair, Seventh Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII), Tokyo, Japan, September 2-8, 2011.
Session Chair, Sixteenth International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XVI, Kanazawa, Japan, September 11-17, 2011.
Session Chair, An International Symposium “Recent Advances on Many Electron Theories II, 2011,” Puri, Orissa, India, December 1-4, 2011.
Session Chair, The Fifth Asian Pacific Conference of Theoretical and Computational Chemistry (APCTCC 2011), Rotorua, New Zealand, December 9-13, 2011.
Session Chair, 6th Conference “Current Trends in Theoretical Chemistry” (CTTC VI), Cracow, Poland, September 1-5, 2013.
Session Chair, Eighteenth International Workshop on Quantum Systems in Chemistry, Physics, and Biology, QSCP-XVIII, Paraty (Rio de Janeiro), Brazil, December 1-7, 2013.
Session Chair, Nordita program on “Computational Challenges in Nuclear and Many-Body Physics,” Stockholm, Sweden, September 15 - October 10, 2014.
Session Chair, Tenth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2014), Santiago, Chile, October 5-10, 2014.
Session Chair, Workshop of the Espace de Structure Nucléaire Théorique on “Near-Degenerate Systems in Nuclear Structure and Quantum Chemistry from Ab-Initio Many-Body Methods,”

CEA Saclay, France, March 30 - April 2, 2015.

Session Chair, 35th Annual Combustion Research Meeting, Bolger Center, Potomac, Maryland, U.S.A., May 26-29, 2015.

Session Chair, 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.

Session Chair, 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.

Session Chair, The symposium “Recent Progress in Molecular Theory for Excited-State Electronic Structure and Dynamics” at the 2015 International Chemical Congress of Pacific Basin Societies (Pacifichem 2015), Honolulu, Hawaii, U.S.A., December 15-20, 2015.

Session Chair, TSRC Workshop “Low-Scaling and Unconventional Electronic Structure Techniques” (LUEST 2016), 3rd edition, Telluride, Colorado, U.S.A., June 1-5, 2016.

Session Chair, Symposium on Electronic Structure Theory (entitled “Advances in Electron Correlation: From Strongly Correlated to Large Systems”) during the Ninth Congress of the International Society for Theoretical Chemical Physics (ISTCP-IX), Grand Forks, North Dakota, U.S.A., July 17-22, 2016.

Session Chair, TSRC Workshop “Low-Scaling and Unconventional Electronic Structure Techniques” (LUEST 2018), 4th edition, Telluride, Colorado, U.S.A., June 4-8, 2018.

Session Chair, 8th Conference “Current Trends in Theoretical Chemistry” (CTTC VIII), Cracow, Poland, September 1-4, 2019.

Session Chair, The Utah Workshop on Quantum Methods in Molecular and Solid-State Theory, Park City, Utah, U.S.A., September 22-27, 2019.

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

Session Chair, the “Quantum International Frontiers 2019” conference, Shanghai, China, November 18-22, 2019.

Session Chair, Virtual TSRC Workshop “Low-Scaling and Unconventional Electronic Structure Techniques” (LUEST 2020), 5th edition, Telluride, Colorado, U.S.A., June 1-5 and June 8-9, 2020.

Session Chair, Hybrid TSRC Workshop “New Developments in Coupled-Cluster Theory,” 4th edition, Telluride, Colorado, U.S.A., July 19-23, 2021.

Session Chair, Modeling and Design of Molecular Materials 2022 (MDMM 2022) Conference, Gdańsk, Poland, September 19-22, 2022.

Session Chair, The 5th Conference on Theory and Applications of Computational Chemistry (TACC 2023), Sapporo, Japan, September 4-9, 2023.

Referee for *Science*, *Physical Review Letters*, *Physical Review A*, *Physical Review B*, *Physical Review C*, *Physical Review E*, *Chemical Physics Letters*, *Chemical Physics*, *Journal of Chemical Physics*, *Journal of Applied Physics*, *Molecular Physics*, *Computer Physics Communications*, *European Physics Journal A*, *European Physics Journal D*, *SIAM Journal on Applied Algebra and Geometry*, *Theoretica Chimica Acta*, *Theoretical Chemistry Accounts*, *International Journal of Quantum Chemistry*, *Journal of Chemical Theory and Computation*, *Journal of Molecular Structure (THEOCHEM)*, *Journal of Computational Chemistry*, *Physical Chemistry Chemical Physics*, *Journal of Physical Chemistry Letters*, *Journal of Physical Chemistry A*, *Journal of the American Chemical Society*, *Organometallics*, *Chemical Science*, *Canadian Journal of Chemistry*, *New Journal of Chemistry*, *Collection of Czechoslovak Chemical Communications*, *Spectroscopy Letters*, *Pramana*, *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 *Grant Agency at the Academy of Sciences of the Czech Republic*, the *National Science Centre* (Poland), the *Danish Council for Independent Research*, the *Icelandic Research Fund*, and the *Swiss National Supercomputing Centre (CSCS)*.

Member of the US Department of Energy (DOE) Theory, Modeling, and Simulation in Nanoscience Review Panel in 2003, panelist at the DOE Office of Science Workshop on Computational Materials Science and Chemistry for Innovation in 2010, on-site reviewer of the Chemical Dynamics in the Gas Phase Program at Argonne National Laboratory, in 2010 and 2016, panel member for a joint Council for Chemical Research and Department of Energy workshop, entitled “Harnessing DOE’s High Performance Computing Expertise to Strengthen the US Chemical Enterprise,” in 2011, and member of review panels for the Chemical Theory, Models, and Computational Methods program at the National Science Foundation (2012/2013, 2021, 2022).

Member of the Selection Committee for one of the American Chemical Society National Awards (2013–2015; chair, 2015).

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

- *Department of Chemistry*

Member of the Chemistry Department Computer Committee, 1998–2018

Chair of the Chemistry Department Computer Committee, 2000–2003

Member of the Chemistry Department Graduate Admissions Committee, 2003/2004, 2023/2024

Member of the Chemistry Department Graduate Advising Committee, 2004/2005

Member of the Chemistry Department Reappointment and Promotion Committee, 2008/2009, 2013/2014, 2016/2017

Chair of the Chemistry Department Reappointment and Promotion Committee, 2016/2017

Member of the Chemistry Department Academic Competitiveness Committee, 2014/2015

Member of the Chemistry Department Colloquium Committee, 2018–2023

Chair of the Chemistry Department Colloquium Committee, 2020/2021, 2021/2022

Member of the Office Supervisor II Search Committee, 2019

Member of the Chemistry Department Information Technology Committee, 2020–present

Chair of Search Committee for an Opportunity Hire in Theoretical Chemistry, 2023

- *College of Natural Science*

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

Member of the Complex Materials Faculty Search Committee, 2010/2011

- *University*

Member of the University Appeals Board, 2001–2007

Co-founder and Member of the Advisory Committee of the High Performance Computing Center, 2004–2009

Member of the Mesoscopic Theory Center, 2006–present

Instructor for the Frontiers in Science Weekend Workshop series for Secondary Science Teachers, 2007

Member of Visioning Committee for Cyber Enabled Discovery, 2008

Member of the Leadership Team for Institute for Cyber Enabled Research, 2008

Member of the Organizing Committee for the Union of Tenure System Faculty at Michigan State University, 2023–present

Other Examples of Synergistic Activities

Co-author of the electronic structure package GAMESS (coupled-cluster, equation-of-motion coupled-cluster, and cluster-in-molecule coupled-cluster and many-body perturbation theory codes; user base of over 150,000 in more than 100 countries).

Co-author of the open-source CCT3 (plugin to PSI4), CCpy, Minicpy, and ccq quantum chemistry software packages on GitHub.

Contributor of potential energy surfaces to the on-line library POTLIB.
Creator of online lecture series entitled “Algebraic and Diagrammatic Methods for Many-Fermion Systems,” consisting of more than 40 HD videos based on CHEM 580 and PHYSICS 580 graduate course offered at Washington University in St. Louis (WUSTL) during research leave in Spring 2016, recorded by the Teaching Center at WUSTL (offered also to students at Michigan State University via video-recorded lectures and online materials), available on YouTube (https://www.youtube.com/results?search_query=Chem+580+Piecuch&sp=CAM%253D; search for ‘Chem 580 Piecuch’).

Press Releases, Popular Feature Articles, and Other Facts Highlighting 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!* and *Phys.org*, March 14, 2007, “Beyond the nuclear shell model,” *Physics Today*, November 2007, and dozens of other articles have discussed our nuclear structure coupled-cluster effort [inspired by our article M. Horoi, J.R. Gour, M. Włoch, M.D. Ludriquito, B.A. Brown, and P. Piecuch, “Coupled-Cluster and Configuration-Interaction Calculations for Heavy Nuclei,” *Phys. Rev. Lett.* **98**, 112501-1 – 112501-4 (2007) and, in part, by the Michigan State University news releases, such as “Physicists wipe away complexity for a clearer view of atomic nuclei” published by *MSU Today* on March 15, 2007].

An article C.J. Cramer, M. Włoch, P. Piecuch, C. Puzzarini, and L. Gagliardi, *J. Phys. Chem. A* **110**, 1991-2004 (2006) was recognized as one of the “Most-Cited Articles Published in 2006” in *The Journal of Physical Chemistry A*.

The Air Force Office of Scientific Research STTR 09.B solicitation calling for proposals on Coupled Cluster Methods for Multi-Reference Applications (AF09-BT40) 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.

An article W. Li, P. Piecuch, J.R. Gour, and S. Li, *J. Chem. Phys.* **131**, 114109-1–114109-30 (2009) was selected for the October 5, 2009 issue of *Virtual Journal of Nanoscale Science & Technology* and the October 1, 2009 issue of *Virtual Journal of Biological Physics Research*, published in the past by the American Institute of Physics and the American Physical Society in cooperation with other societies and publishers.

An article J.A. Hansen, P. Piecuch, and B.G. Levine, “Communication: Determining the Lowest-Energy Isomer of Aug: 2D, or not 2D,” *J. Chem. Phys.* **139**, 091101-1 – 091101-4 (2013) was identified by *The Journal of Chemical Physics* as one of the Top 20 Most Read articles in September 2013.

One of our most frequently cited articles, P. Piecuch and M. Włoch, “Renormalized Coupled-Cluster Methods Exploiting Left Eigenstates of the Similarity-Transformed Hamiltonian,” *J. Chem. Phys.* **123**, 224105-1–224105-10 (2005), was identified by *Thomson Reuters Web of Science* as a Highly Cited Paper. According to *Web of Science*, as of January/February 2015 and in selected time periods afterwards, this paper received enough citations to place it in the top 1 % of its academic field based on a highly cited threshold for the field and publication year (data taken from *Thomson Reuters Essential Science Indicators*).

The Michigan State University news releases published by *MSU Today* (January 12, 2018) and MSU’s College of Natural Science (December 20, 2017), entitled “Quantum Leap: Novel Computational Approach Launches New Paradigm in Electronic Structure Theory,” which discuss the significance of our article J.E. Deustua, J. Shen, and P. Piecuch, “Converging High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions,” *Phys. Rev. Lett.* **119**, 223003-1 – 223003-5 (2017), were posted as a University Research Highlight on the US Department of Energy Office of Science homepage (see the ‘University and Stakeholder News’ section, note dated December 21, 2017) and in *Phys.org* (December

22, 2017), *AAAS EurekAlert!* (January 12, 2018), and several other media outlets. Our *Science Advances* article S.H. Yuwono, I. Magoulas, and P. Piecuch, “Quantum Computation Solves a Half-Century-Old Enigma: Elusive Vibrational States of Magnesium Dimer Found,” *Sci. Adv.* **6**, eaay4058 (2020) has been featured by *Phys.org* (April 13, 2020; “Quantum computation solves an old enigma: Finding the vibrational states of magnesium dimer” by Thamarasee Jeewandara) and several other media outlets. The Michigan State University news releases published by *MSU Today* (May 11, 2020) and MSU’s College of Natural Science (May 11, 2020), entitled “MSU Scientists Solve Half-Century-Old Magnesium Dimer Mystery,” which discuss the significance of the research reported in this article, were posted in *AAAS EurekAlert!* (May 22, 2020) and publicized in other science news outlets as well. In particular, the *MSU Today* article was highlighted on the US Department of Energy Office of Science homepage (see the “University and Stakeholder News” section, note dated June 4, 2020).

Our paper J. Lahiri, M. Moemeni, I. Magoulas, S.H. Yuwono, J. Kline, B. Borhan, P. Piecuch, J.E. Jackson, G.J. Blanchard, and M. Dantus, “Steric Effects in Light-Induced Solvent Proton Abstraction,” *Phys. Chem. Chem. Phys.* **22**, 19613-19622 (2020) has been selected by the Editors of *Phys. Chem. Chem. Phys.* as a 2020 HOT PCCP article.

Our article, G.M.J. Barca, C. Bertoni, L. Carrington, D. Datta, N. De Silva, J.E. Deustua, D.G. Fedorov, J.R. Gour, A.O. Gunina, E. Guidez, T. Harville, S. Irle, J. Ivanic, K. Kowalski, S.S. Leang, H. Li, W. Li, J.J. Lutz, I. Magoulas, J. Mato, V. Mironov, H. Nakata, B.Q. Pham, P. Piecuch, D. Poole, S.R. Pruitt, A.P. Rendell, L.B. Roskop, K. Ruedenberg, T. Sattasathuchana, M.W. Schmidt, J. Shen, L. Slipchenko, M. Sosonkina, V. Sundriyal, A. Tiwari, J.L.G. Vallejo, B. Westheimer, M. Włoch, P. Xu, F. Zahariev, and M.S. Gordon, “Recent Developments in the General Atomic and Molecular Electronic Structure System,” *J. Chem. Phys.* **152**, 154102-1 – 154102-26 (2020), has been identified by *Web of Science* as a Highly Cited Paper. According to *Web of Science*, as of November/December 2020 and in more recent months (most recently, May/June 2023), this paper received enough citations to place it in the top 1 % of its academic field based on a highly cited threshold for the field and publication year. *Web of Science* has also identified it as a Hot Paper, i.e., the paper that in November/December 2020 and in more recent months (most recently, January/February 2022) and within two years of its publication date received enough citations to place it in the top 0.1 % of papers in its academic field (data taken from *Essential Science Indicators*).

Our paper W. Park, J. Shen, S. Lee, P. Piecuch, M. Filatov, and C.H. Choi, “Internal Conversion between Bright ($1^1B_u^+$) and Dark ($2^1A_g^-$) States in *s-trans*-Butadiene and *s-trans*-Hexatriene,” *J. Phys. Chem. Lett.* **12**, 9720-9729 (2021) has been selected for a supplementary cover in the October 7th, 2021 issue of *J. Phys. Chem. Lett.* MSU’s College of Natural Science published a news story about it, entitled “MSU Chemistry Article Honored with Supplementary Cover,” on November 16, 2021.

Our invited article S.H. Yuwono, A. Chakraborty, J.E. Deustua, J. Shen, and P. Piecuch, “Accelerating Convergence of Equation-of-Motion Coupled-Cluster Computations Using the Semi-Stochastic CC($P;Q$) Formalism,” *Mol. Phys.* **118**, e1817592 (2020) (17 pages; included in the Special Issue of *Molecular Physics* in Honour of Professor Jürgen Gauss) has been chosen by the panel of Editors as the best paper published in *Mol. Phys.* in 2020. As a result, Stephen Yuwono has also been awarded the 2020 Longuet-Higgins Early Career Researcher Prize. For more information, see the articles G. Jackson (Chairman of the Editors), “Announcement of the Winner of the Longuet-Higgins Early Career Researcher Prize 2020,” *Mol. Phys.* **119**, e2010864 (2021) and “Molecular Physics Longuet-Higgins Early Career Researcher Prize 2020 Winner’s Profile,” *Mol. Phys.* **119**, e2003963 (2021). See, also, the MSU’s College of Natural Science news story, published on December 14, 2021, entitled “Chemistry Graduate Student Wins Prestigious Early Career Award.”

Our article J. Lahiri, S.H. Yuwono, I. Magoulas, M. Moemeni, B. Borhan, G.J. Blanchard, P. Piecuch, and M. Dantus, “Controlling Quantum Interference between Virtual and Dipole Two-Photon Optical Excitation Pathways Using Phase-Shaped Laser Pulses,” *J. Phys. Chem. A* **125**, 7534-7544 (2021) has been included in a *Virtual Issue of the Journal of Physical Chemistry A* entitled “A Venue for Advances in Experimental and Theoretical Methods in Physical

Chemistry.” For more information about it, see the preface by A.J. Orr-Ewing, T.D. Crawford, M.T. Zanni, G. Hartland, and J.-E. Shea, *J. Phys. Chem. A* **126**, 177 (2022).

Our paper W. Park, J. Shen, S. Lee, P. Piecuch, T. Joo, M. Filatov (Gulak), and C.H. Choi, “Dual Fluorescence of Octatetraene Hints at a Novel Type of Singlet-to-Singlet Thermally Activated Delayed Fluorescence Process,” *J. Phys. Chem. C* **126**, 14976-14985 (2022) has been selected for a supplementary cover in the September 8th, 2022 issue of *J. Phys. Chem. C*.

Our invited PCCP Perspective, included in a Themed Collection PCCP Reviews, A.M. Teale, T. Helgaker, A. Savin, C. Adamo, B. Aradi, A.V. Arbuznikov, P.W. Ayers, E.J. Baerends, V. Barone, P. Calaminici, E. Cancès, E.A. Carter, P.K. Chattaraj, H. Chermette, I. Ciofini, T.D. Crawford, F. De Proft, J.F. Dobson, C. Draxl, T. Frauenheim, E. Fromager, P. Fuentealba, L. Gagliardi, G. Galli, J. Gao, P. Geerlings, N. Gidopoulos, P.M.W. Gill, P. Gori-Giorgi, A. Görling, T. Gould, S. Grimme, O. Gritsenko, H.J.A. Jensen, E.R. Johnson, R.O. Jones, M. Kaupp, A.M. Köster, L. Kronik, A.I. Krylov, S. Kvaal, A. Laestadius, M. Levy, M. Lewin, S. Liu, P.-F. Loos, N.T. Maitra, F. Neese, J.P. Perdew, K. Pernal, P. Pernet, P. Piecuch, E. Rebolini, L. Reining, P. Romaniello, A. Ruzsinszky, D.R. Salahub, M. Scheffler, P. Schwerdtfeger, V.N. Staroverov, J. Sun, E. Tellgren, D.J. Tozer, S.B. Trickey, C.A. Ullrich, A. Vela, G. Vignale, T.A. Wesolowski, X. Xu, and W. Yang, “DFT Exchange: Sharing Perspectives on the Workhorse of Quantum Chemistry and Materials Science,” *Phys. Chem. Chem. Phys.* **24**, 28700-28781 (2022) has been selected by the Editors of *Phys. Chem. Chem. Phys.* as a 2022 HOT PCCP article and for a cover in the December 21st, 2022 issue of *Phys. Chem. Chem. Phys.* It has also been identified by *Web of Science* as a Highly Cited Paper. According to *Web of Science*, as of May/June 2023, this paper received enough citations to place it in the top 1 % of its academic field based on a highly cited threshold for the field and publication year (data taken from *Essential Science Indicators*).

Professional Societies

European Academy of Sciences, Arts, and Humanities (Paris, France; Elected Corresponding Member since 2003), International Academy of Quantum Molecular Science (Menton, France; Elected Member since 2018), American Physical Society (Regular Member since 1999, Fellow since 2008), American Chemical Society (Regular Member since 1996), American Association for the Advancement of Science (Professional Member since 2008, Fellow since 2011), Royal Society of Chemistry (Fellow since 2016), International Society for Theoretical Chemical Physics (Regular Member since 1994), World Association of Theoretical and Computational Chemists (Regular Member since 1990, Life Member since 2005), FRIB Theory Alliance (Member since 2023).