

Curriculum Vitae of Monika Musiał

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Education:

M.Sc. degree: 1996, Institute of Chemistry, University of Silesia
Katowice, Poland
Ph.D. degree: 2002, Institute of Chemistry, University of Silesia
Katowice, Poland (with distinction)
Habilitation: 2010, Department of Chemistry, University of Warsaw
Warsaw, Poland (with distinction)
Professor: 2014, Institute of Chemistry, University of Silesia
Katowice, Poland

Employment:

2000 – 2004 Teaching and Research Assistant, Institute of Chemistry, University of Silesia
2004 – 2010 Assistant Professor, Institute of Chemistry, University of Silesia
2011 – 2013 Associate Professor, Institute of Chemistry, University of Silesia
2014 – Professor of Chemistry, Institute of Chemistry, University of Silesia

Teaching experience:

- quantum and theoretical chemistry courses for chemistry students
- monograph lectures:

Coupled Cluster Method

Diagrammatic methods in quantum chemistry

Ionized and Excited States of Atoms and Molecules

New methods to study excited states of atoms and molecules

Molecular properties for the Coupled Cluster (CC) and
Equation-of-Motion CC methods

Editing and co-authorship of the two textbooks for students in the field of quantum chemistry.

Supervision of Master's theses (26 completed) and Bachelors's theses (43 completed).

International experience:

2000	Scientific visit to University of Florida, Quantum Theory Project, Gainesville, FL, USA
2002 – 2003	Postdoctoral Research Associate, University of Florida, Gainesville, FL, USA
2004 – 2015	Visiting Professor, University of Florida, Gainesville, FL, USA (over 15 2-3 months visits)
2007	Visiting Scientist, Laboratoire de Chimie, Quantique Université Louis Pasteur, Strasbourg, France
2008	Visiting Scientist, Institute for Nuclear Theory, University of Washington, Seattle, WA, USA

Research areas:

- quantum chemical methods including electron correlation
- accurate calculation of molecular properties
- coupled cluster method for atoms and molecules

Development of the new computational methods aimed at the determination of energetic effects accompanying bond breaking processes. The new schemes rely on the highly elaborate approach to the evaluation of electronic correlation effects based on the coupled cluster method. These computational tools are particularly useful in studies of potential energy curves and owing to that they can be used in the accurate description of a dissociation process. Such very accurate methods are necessary in the studies of molecules in ultralow temperatures where the precise knowledge of interatomic interactions in the whole range of the distance between engaged atoms is required. The application power of these studies is enormous, e.g. a high precision spectroscopy, quantum computers, superaccurate determination of the fundamental physical constants, etc..

Encouraging results are obtained in the studies of the alkali metal diatomics via (2,0) sector of Fock space coupled cluster method (M. Musiał, *J. Chem. Phys.*, **136**, 134111 (2012)) (i.e., indirect applications of the double electron attachment - DEA - quantity) for the precise knowledge of the interatomic potentials which is crucial, e.g., in the design of the synthesis of molecules in the ultra low temperatures. E.g., our results for the potential

energy curves of the Rubidium dimer were utilized in the studies of the optimal reaction path of the Rb_2 molecules (M. Tomza, M. H. Goerz, M. Musiał, R. Moszynski, Ch. P. Koch, *Phys. Rev. A*, **86**, 043424 (2012)).

Developing various realizations of the Fock space coupled cluster approaches (EE - excitation energy, EA - electron affinity, IP - ionization potential, DEA - double electron affinity, DIP - double ionization potential, TEA - triple electron affinity), new computational strategies to calculate excited states of systems are proposed. Same refers to the equation-of-motion coupled cluster theory.

Research grants, awards, distinctions:

- 2005-2015 Nine individual awards granted by the Rector of the University of Silesia
- 2000-2001 Main grant researcher (supported by the Committee for Scientific Research)
- 2003-2005 Main grant researcher (supported by the Committee for Scientific Research)
- 2008-2009 Recipient of the habilitation grant from the Ministry of Science and Higher Education of Poland
- 2010-2011 Recipient of the individual grant from the Ministry of Science and Higher Education of Poland
- 2012-2013 Recipient of the individual grant from the National Science Centre, Poland
- 2013-2016 Recipient of the individual grant from the National Science Centre, Poland
- 2020-2025 Vice-coordinator Priority Research Areas: *Fundamental and universal properties of the nature* via Research Excellence Initiative of the University of Silesia in Katowice
- 2012-2019 Vice-chair of the Polish Chemical Society (Theoretical Chemistry Section)

- 2019-2022 Chair of the Polish Chemical Society (Theoretical Chemistry Section)

Scientific achievements:

- papers published: 92
- citations: 8802 (Google Scholar)
- expert at the European Research Council (ERC), PE4 Panel (Physical and Analytical Chemical Sciences), for the evaluation of the CoG-2024 Consolidator Grant
- co-author of the wellknown quantum chemistry program packages: ACESII and GAMESS
- from 2023 Editorial Board Member: *Advances in Quantum Chemistry*, Academic Press
- most cited paper: R. J. Bartlett, M. Musiał, *Rev. Mod. Phys.*, 79, 291 (2007) – 3948 (Google Scholar) citations (IF=38.4)
- co-authorship of the review article discussing the multireference nature of the chemical bond published in one of the top chemistry journals *Chemical Reviews* (IF=41.3, 601 citations (Google Scholar))
- authorship of the chapter *Equation-of-motion coupled cluster models* in *Quantum Chemistry and Dynamics of Excited States*, Leticia Gonzales and Roland Lindh (eds.), John Wiley and Sons Ltd (2020)
- co-editor *Advances in Quantum Chemistry - New electron correlation methods and their applications, and use of atomic orbitals with exponential asymptotes* (Academic Press 2021)
- co-editor *Advances in Quantum Chemistry - Polish Quantum Chemistry from Kołos to now* (Academic Press 2023)
- member/reviewer of several research funding committees (Polish and foreign)

- reviewer in doctoral, habilitation assesment processes and in processes for the conferment of the title of *professor*
- peer review for scientific journals, e.g., *Nature Communications*, *Journal of Physical Chemistry Letters*, *Journal of Chemical Physics*, *Journal of Chemical Theory and Computation*, *Physical Chemistry Chemical Physics*, *Journal of Physical Chemistry A*, *Chemical Physics Letters*, *Molecular Physics*, *Advances in Quantum Chemistry*
- organization of international conferences, e.g., *15th Central European Symposium on Theoretical Chemistry* (Poland, September 2017); co-chair with Prof. Krzysztof Pachucki - *Warsaw Molecular Electronic Structure Virtual Conference*, (Poland, September 2020)
- membership of the Scientific Committee organizing *the Utah Workshop on Methods and Applications in Molecular and Solid State Theory* (September 2019)
- membership of the Scientific Committee organizing *Molecular Electronic Structure Conferences*
- membership of the Scientific Committee organizing *Central European Symposiums on Theoretical Chemistry*
- chair of the Theoretical Chemistry Section as a part of the 62nd ceremonial conference of Polish Chemical Society (September 2019) in Warsaw (Poland) with Prof. Robert Moszyński from University of Warsaw
- over 145 conference presentations, 36 invited lectures at various conferences, e.g. during:
 - *International Society for Theoretical Chemical Physics Conference*, Slovakia
 - *International Congress of Quantum Chemistry*, USA
 - *Sanibel Symposiums*, USA
 - *Regional Meeting on the American Chemical Society*, USA
 - *Symposium of 50 Years of Coupled Cluster*, USA
 - *EMN (Energy, Materials and Nanotechnology) Meeting on Computation and Theory*, USA
 - *International Society for Theoretical Chemical Physics Conference*, USA

- *Energy Materials Nanotechnology Meeting on Computation and Theory*, Dubai, UAE
 - *Molecular Electronic Structure Conferences*, Turkey, France, Argentina, Tunisia, Italy
 - *ESNT workshop on near degenerate systems in nuclear structure and quantum chemistry from ab initio many-body methods*, France
 - *Recent Advances in Many-Electron Theories*, India
 - *Central European Symposium on Theoretical Chemistry*, Slovakia
 - *International Conference of Computational Methods in Sciences and Engineering*, Greece
 - *The Systematic Treatment of Electron Correlation. A Celebration of the Science of Rodney J. Bartlett*, USA
 - *Quantum Chemistry Workshop*, Poland
 - *Current Trends in Theoretical Chemistry Conferences*, Poland
 - *Polish Chemical Society Meetings*, Poland
- supervision of PhD dissertations (5 completed)
 - Hirsch h-index: 36 (Google Scholar)