Paweł Tecmer

Ph.D.

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87-100, Toruń, Poland
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Institute of Physics
Nicolaus Copernicus University in Toruń

Curriculum Vitae

Personal Data

Nationality	polish
Place of birth	Kwidzyn, Poland
Date of birth	15 April 1983

Work Experience

09.2016–present	**postdoctoral fellow**, *Nicolaus Copernicus University in Toruń*, Toruń, Poland.
04.2016–08.2016	**research assistant**, *Nicolaus Copernicus University in Toruń*, Toruń, Poland.
01.2016–03.2016	**researcher/visiting professor**, *Nicolaus Copernicus University in Toruń*, Toruń, Poland.
07.2013–12.2015	**postdoctoral fellow**, *McMaster University*, Hamilton, Canada.
07.2012–06.2013	**postdoctoral fellow**, *ETH Zürich*, Zürich, Switzerland.

Education

06.2008–06.2012	**Ph.D.**, *VU University Amsterdam*, Amsterdam, The Netherlands.
09.2006–05.2008	**Master**, *Nicolaus Copernicus University in Toruń*, Toruń, Poland.
09.2003–06.2006	**Bachelor**, *Nicolaus Copernicus University in Toruń*, Toruń, Poland.
09.1998–05.2003	**Agribusiness Lyceum (high school)**, Kwidzyn, Poland.
09.1997–05.2000	**Diploma in music education (clarinet)**, Kwidzyn, Poland.

PhD Project

Title	*Towards reliable modeling of excited states of uranium compounds.*
Supervisor	Prof. Lucas Visscher

Master Project

Title	*Relativistic basis sets for the 2-nd and 18-th group elements optimized for the infinite-order two-component (IOTC) Hamiltonian.*
Supervisors	Prof. M. Barysz and Prof. M. Klobukowski

Publications

22 **Katharina Boguslawski and Paweł Tecmer**, *Benchmark of Dynamic Electron Correlation Models for Seniority-Zero Wavefunctions and Their Application to Thermochemistry*, *arXiv:*, 2016, *submitted to J. Chem. Theory Comput.*

22 **Katharina Boguslawski, Florent Réal, Paweł Tecmer, Corinne Duperrouzel, André S. P. Gomes, Örs Legeza, Paul W. Ayers, and Valérie Vallet**, *On the Multi-Reference Nature of Plutonium Oxides: PuO_2^{2+}, PuO_2, PuO_3 and $PuO_2(OH)_2$*, *arXiv:1608.02353*, 2016, *submitted to Phys. Chem. Chem. Phys.*

21 **Katharina Boguslawski, Paweł Tecmer, and Örs Legeza**, *Analysis of Two-Orbital Correlations in Wavefunctions Restricted to Electron-Pair States*, *arXiv:1606.08503*, 2016, *submitted to Phys. Rev. B.*

20 **Paweł Tecmer, Sung W. Hong, and Katharina Boguslawski**, *Dissecting the Cation–Cation Interaction between Two Uranyl Units*, *Phys. Chem. Chem. Phys.*, 2016, **18**, 18305–18311.

19 **Daniel Stuart, Paweł Tecmer, Paul W. Ayers, and Katharina Boguslawski**, *The Effect of Nitrido, Azide, and Nitrosyl Ligands on Magnetization Densities and Magnetic Properties of Iridium PNP Pincer-Type Complexes*, *RSC Adv.*, 2015, **5**, 84311–84320.

18 **Yilin Zhao, Katharina Boguslawski, Paweł Tecmer, Corinne Duperrouzel, Gergely Barcza, Örs Legeza, and Paul W. Ayers**, *Dissecting the Bond-formation Process of d 10-Metal-Ethene Complexes with Multireference Approaches*, *Theor. Chem. Acc.*, 2015, **134**, 120.

17 **Paweł Tecmer, Katharina Boguslawski, and Paul W. Ayers**, *Singlet Ground State Actinide Chemistry with Geminals*, *Phys. Chem. Chem. Phys.*, 2015, **17**, 14427–14436.

16 **Katharina Boguslawski and Paweł Tecmer**, *Orbital Entanglement in Quantum Chemistry*, *Int. J. Quantum Chem.*, 2015, **115**, 1289–1295.

15 **Corinne Duperrouzel, Paweł Tecmer, Katharina Boguslawski, Gergely Barcza, Örs Legeza, and Paul W. Ayers**, *A quantum Informational Approach for Dissecting Chemical Reactions*, *Chem. Phys. Lett.*, 2015, **621**, 160–164.

14 **Katharina Boguslawski, Paweł Tecmer, Patrick Bultinck, Stijn De Baerdemacker, Dimitri Van Neck, and Paul W. Ayers**, *Non-variational Orbital Optimization Techniques for the AP1roG Wave Function*, *J. Chem. Theory. Comput.*, 2014, **10**, 4873–4882.

13 **Paweł Tecmer, André S. P. Gomes, Stefan Knecht, and Lucas Visscher**, *Relativistic Fock-Space Coupled Cluster Study of Small Building Blocks of Larger Uranium Complexes*, *J. Chem. Phys.*, 2014, **141**, 041107.

12 **Paweł Tecmer, Katharina Boguslawski, Paul A. Johnson, Peter A. Limacher, Matthew Chan, Toon Verstraelen, and Paul W. Ayers**, *Assessing the Accuracy of New Geminal-Based Approaches*, *J. Phys. Chem. A*, 2014, **118**, 9058–9068.

11 **Katharina Boguslawski, Paweł Tecmer, Peter A. Limacher, Paul A. Johnson, Paul W. Ayers, Patrick Bultinck, Stijn De Baerdemacker, and Dimitri Van Neck**, *Projected Seniority-Two Orbital Optimization of the Antisymmetric Product of One-Reference Orbital Geminal*, *J. Chem. Phys.*, 2014, **140**, 214114.

10 **Katharina Boguslawski, Paweł Tecmer, Paul W. Ayers, Patrick Bultinck, Stijn De Baerdemacker, and Dimitri Van Neck**, *Efficient Description of Strongly Correlated Electrons with Mean-Field Cost*, *Phys. Rev. B*, 2014, **89**, 201106(R).

9 **Matthieu Mottet, Paweł Tecmer, Katharina Boguslawski, Örs Legeza, and Markus Reiher**, *Quantum Entanglement in Carbon-Carbon, Carbon-Phosphorus and Silicon-Silicon Bonds*, *Phys. Chem. Chem. Phys.*, 2014, **16**, 8872–8880.

8 **Paweł Tecmer, Katharina Boguslawski, Örs Legeza, and Markus Reiher**, *Unravelling the Quantum-Entanglement Effect of Noble Gas Coordination on the Spin Ground State of CUO*, *Phys. Chem. Chem. Phys.*, 2014, **16**, 719–727.

7 **Mateusz Borkowski, Piotr Żuchowski, Roman Ciuryło, Paul Julienne, Dariusz Kędziera, Łukasz Mentel, Paweł Tecmer, Frank Münchow, Cristian Bruni, and Axel Görlitz**, *Scattering Lengths in Isotopologues of the RbYb System*, *Phys. Rev. A*, 2013, **88**, 052708.

6 **Paweł Tecmer, Niranjan Govind, Karol Kowalski, Lucas Visscher, and Wibe A. de Jong**, *Reliable Modeling of the Electronic Spectra of Realistic Uranium Complexes*, *J. Chem. Phys.*, 2013, **139**, 034301.

5 **Katharina Boguslawski, Paweł Tecmer, Gergely Barcza, Örs Legeza, and Markus Reiher**, *Orbital Entanglement in Bond-Formation Processes*, *J. Chem. Theory Comput.*, 2013, **9**, 2959–2973.

4 **Katharina Boguslawski, Paweł Tecmer, Örs Legeza, and Markus Reiher**, *Entanglement Measures for Single- and Multi-Reference Correlation Effects*, *J. Phys. Chem. Lett.*, 2012, **3**, 3129–3135.

3 **Paweł Tecmer, Henk van Lingen, André S. P. Gomes, and Lucas Visscher**, *The Electronic Spectrum of CUONg4 (Ng = Ne, Ar, Kr, Xe): New Insights in the Interaction of the CUO Molecule with Noble Gas Matrices*, *J. Chem. Phys*, 2012, **37**, 084308.

2 **Paweł Tecmer, Radovan Bast, Kenneth Ruud, and Lucas Visscher**, *Charge Transfer Excitations in Uranyl Tetrachloride ($[UO_2Cl_4]^{2-}$): How Reliable is the Electronic Spectrum from Relativistic Time-Dependent Density Functional Theory?*, *J. Phys. Chem. A*, 2012, **116**, 7397–7404.

1 **Paweł Tecmer, André S. P. Gomes, Ulf Ekström, and Lucas Visscher**, *Electronic Spectroscopy of UO_2^{2+}, NUO^+ and NUN: An Evaluation of Time-Dependent Density Functional Theory for Actinides*, *Phys. Chem. Chem. Phys.*, 2011, **13**, 6249-6259.

Book chapters (peer-reviewed)

1 **Paweł Tecmer, Katharina Boguslawski, and Dariusz Kędziera**, *Relativistic Methods in Computational Quantum Chemistry*, *in Handbook of Computational Chemistry*, 2016, **vol. 2**, 1–43.

Scientific Visits

01.09–14.09.2015 Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Toruń, Poland

25.05–26.05.2015 PhLAM institute at the University of Lille, Lille, France

11.11–29.11.2013 Center for Molecular Modeling (CMM), Gent University, Gent, Belgium

02.05–03.06.2011 Pacific Northwest National Laboratory (PNNL), Richland, USA

Invited Lectures at Conferences

10–14.10.2016 ENM Meting on Computation and Theory, *Towards reliable modeling of electronic structures and spectroscopic parameters of uranium oxides*, Las Vegas, USA

18.12.2015 Pacifichem 2015, *Large scale modelling of strong electron correlation effects in extended systems from geminals*, Honolulu, USA

16.12.2015 Pacifichem 2015, *Efficient description of electron correlation effects in actinide compounds*, Honolulu, USA

13–14.10.2014 WATOC 2014 Satellite Meeting on Large Condensed and Biological Systems, *Dissecting the mysterious interaction of uranium with noble gases*, Conceptión, Chile

03–04.10.2014 Symposium on New Approaches in Theoretical Chemistry, *Efficient description of strongly correlated electrons*, Santiago, Chile

17–18.12.2013 Methods for Modelling Molecules and Materials (M4), *Towards efficient description of strongly correlated electrons*, Hamilton, Canada

Other Invited Lectures

08.06.2016 Seminar "Coherence-Correlations-Complexity", Institute of Physics, Wroclaw University of Technology, *Two-electron functions as alternative models for strongly correlated systems*, Wrocław, Poland

09.09.2015 Special Colloquium, Department of Quantum Physics, Nicolaus Copernicus University in Toruń, *Alternative approaches to model strongly correlated systems*, Toruń, Poland

27.05.2015 Theoretical Chemistry Seminar at the VU University Amsterdam, *Alternative approaches to model and interpret strongly correlated systems*, Amsterdam, The Netherlands

26.05.2015 Theoretical Chemistry Seminar at the PhLAM institute at the University of Lille, *Breaking the course of dimension using two-electron functions*, Lille, France

07.11.2013 'Canada Days Workshop' at the Gent University, *Geminals related projects. Past, present and future perspectives*, Ghent, Belgium

27.03.2012 Theoretical Chemistry Seminar, ETH Zürich, *Electronic spectroscopy of uranium-containing complexes*, Zürich, Switzerland

Contributed Lectures and Posters at Conferences

04–09.09.2016 CTTC VII, *(talk: Electron correlation effects in actinide compounds from unconventional wavefunction-based methods)*, Krakow, Poland

16–20.06.2015 ICQC 2015 Satellite Symposium in Kobe *(poster: A quantum informational approach for dissecting chemical reactions)*, Kobe, Japan

08–13.06.2015 15-th International Congress of Quantum Chemistry (15-th ICQC) *(poster: Novel electron correlation methods in actinide chemistry)*, Beijing, China

01–06.06.2015 Recent Advances in Electronic Structure Theory (RAEST) *(poster: Quantum chemistry from two-electron functions: the AP1roG ansatz)*, Nanjing, China

07–09.11.2014 30-th Symposium on Chemical Physics *(talk: Ab initio modeling of excited states of uranium compounds: dissecting the interplay of electron correlation and relativistic effects)*, Waterloo, Canada

05–10.10.2014 10-th Congress of the World Association of Theoretical and Computational Chemists (10-th WATOC) *(poster: New geminal-based approaches in actinide chemistry)*, Santiago, Chile

06–11.07.2014 26-th Canadian Symposium on Theoretical and Computational Chemistry (46-th CSTCC) *(poster: The multi-reference nature of chemistry from geminals)*, Montreal, Canada

21–23.11.2013 Norman March Symposium *(poster: Unravelling the quantum-entanglement effect of noble gas coordination on the ground state of CUO)*, Namur, Belgium

07–08.11.2013 8-th Mathematical Methods for Ab Initio Quantum Chemistry *(poster: Unravelling the quantum-entanglement effect of noble gas coordination on the ground state of CUO)*, Nice, France

01–03.11.2013 29-th Symposium on Chemical Physics *(poster: Unravelling the quantum-entanglement effect of noble gas coordination on the ground state of CUO)*, Waterloo, Canada

26–30.08.2013 Applied Mathematics, Modelling and Computational Science (AMMCS-2013) *(talk: Towards reliable modelling of excited states of actindes from (relativistic) time-dependent density functional theory)*, Waterloo, Canada

02–07.06.2013 7-th Molecular Quantum Mechanics (7-th MQM) *(poster: Entanglement measures for the detection of single- and multi-reference correlation effects)*, Lugano, Switzerland

23–27.09.2012 48-th Symposium on Theoretical Chemistry (48-th STC) *(poster: Entanglement measures for the detection of single- and multi-reference electron correlation effects)*, Karlsruhe, Germany

28–30.11.2011 CHAINS, NWO Symposium *(poster: Large scale modelling of the electronic spectra of uranium-containing molecules: UO_2(saldien) and [UO_2(saldien)]$^-$ in DMSO)*, Utrecht, The Netherlands

21–25.08.2011 47-th Symposium on Theoretical Chemistry (47-th STC) *(poster: Large scale modeling of the electronic spectra of uranium-containing molecules)*, Sursee, Switzerland

17–22.07.2011 9-th Congress of the World Association of Theoretical and Computational Chemists (9-th WATOC) *(poster: Electronic spectroscopy of small actinide molecules: An evaluation of time-dependent density functional theory for actinides)*, Santiago de Compostela, Spain

26–30.09.2010 46-th Symposium on Theoretical Chemistry (46-th STC) *(poster: Electronic spectroscopy of UO_2^{2+}, NUO^+ and NUN: An evaluation of Time-dependent Density Functional Theory)*, Münster, Germany

08–13.06.2009 13-th International Congress of Quantum Chemistry (13-th ICQC) *(poster: Electronic spectroscopy of actinyl ions)*, Helsinki, Finland

19–20.01.2010 NWO Symposium *(poster: Vibrational spectroscopy and electron affinities of uranyl halogens)*, Veldhoven, The Netherlands

27.05–01.06.2009 Very Heavy Metals (VHM) *(talk: Electronic spectroscopy of actinyl ions)*, Canet-Plage, France

26–27.02.2009 NWO Symposium *(poster: Spectroscopy of actinyl ions)*, Lunteren, The Netherlands

Participation in Workshops and Schools

15–17.05.2013 Tensor Network States in Quantum Chemistry, Zürich, Switzerland

04–06.09.2012 Entanglement Based Approaches in Quantum Chemistry, Dresden, Germany

16–20.07.2012 Valence Bond workshop, Paris, France

18–21.06.2012 Annual Dirac developers meeting *(talk1: The electronic spectrum of $CUONg_4$ (Ng = Ne, Ar, Kr, Xe revisited: can this puzzle be solved by Density Functional Theory?; talk2: Charge-transfer excitations in uranyl tetrachloride: how reliable are electronic spectra from relativistic time-dependent density functional theory?)*, Ødense, Denmark

04.11.2011 Holland Research School of Molecular Chemistry Symposium *(poster: Experimental and theoretical study of uranyl halogens)*, Amsterdam, The Netherlands

06–10.12.2010 Winter School for Theoretical Chemistry and Spectroscopy *(talk: Electronic spectroscopy of UO_2^{2+}, NUO^+ and NUN: An evaluation of Time-dependent Density Functional Theory for actinides)*, Han-sur-Lesse, Belgium

25.11.2010 Holland Research School of Molecular Chemistry Symposium *(poster: Electronic spectroscopy of UO_2^{2+}, NUO^+ and NUN: An evaluation of Time-dependent Density Functional Theory)*, Leiden, The Netherlands

31.05–03.06.2010 Annual Dirac developers meeting *(talk: Actinide spectroscopy)*, Ødense, Denmark

07–11.12.2009 Winter School for Theoretical Chemistry and Spectroscopy *(talk: Vibrational spectroscopy and electron affinities of uranyl halogens)*, Han-sur-Lesse, Belgium

09.11.2009 Holland Research School of Molecular Chemistry Symposium *(poster: Electronic transitions in actinyl cations)*, Amsterdam, The Netherlands

06–19.09.2009 European Summer School in Quantum Chemistry, Torre Normana, Sicily, Italy

08–2009 Annual Dirac developers meeting *(talk: Electronic spectroscopy of actinyl ions)*, Ødense, Denmark

05–16.01.2009 MolSim: Understanding Molecular Simulation, Amsterdam, The Netherlands

15–18.12.2008 Winter School for Theoretical Chemistry and Spectroscopy, Han-sur-Lesse, Belgium

27.11.2008 Holland Research School of Molecular Chemistry Symposium *(poster: Electronic spectroscopy of uranyl cation)*, Amsterdam, The Netherlands

Assistance with Conference Organization

02–16.09.2007 Symposium on Advanced Methods of Quantum Chemistry and Physics, Toruń, Poland

Membership in Organizations

06.2008–07.2012 Amsterdam Center for Multiscale Modeling

06.2008–07.2012 Holland Research School of Molecular Chemistry

05.2006–01.2008 Polish Student School of Chemistry

Scholarships/Grants

01.2016–01.2017 Computing Grant from the Wroclaw Center of Networking and Supercomputing

04.2015–03.2017 Travel grant from the France Canada Research Fund (FCRF)

07.2013–06.2016 Executor of the OPUS grant from National Science Centre Poland, project title: *Precise quantum chemistry calculations and dynamic of ultracold molecules*

05.2011–06.2011 The Pacific Northwest National Laboratory Alternate Sponsored Fellowship

09.2002–06.2003 The Polish Minister of Science and Higher Education Scholarship for outstanding achievement in high school

09.2001–06.2002 The Polish Minister of Science and Higher Education Scholarship for outstanding achievement in high school

Student Supervision

10.2015–12.2015 **Sophie Kervazo**, *Computational actinide chemistry*, PhD Student.

05.2015–08.2015 **Corinne Duperrouzel**, *Multireference character of Uranium and Plutonium trioxides*, Summer Student.

05.2014–08.2015 **Hong Sung**, *Cation-cation interactions in actinides*, Summer Student.

09.2014–08.2015 **Yilin Zhao**, *Multi-reference methods in quantum chemistry*, PhD Student.

09.2014–03.2015 **Hong Sung**, *Dissecting the intermolecular interactions between uranyl cations*, Bachelor Student.

09.2014–12.2014 **Daniel Stuart**, *Spin-densities in transition metal complexes*, Coop Student.

05.2014–08.2014 **Corinne Duperrouzel**, *Metal–olefin bonding in nickel-ethylene complexes*, Summer Student.

04.2013–12.2013 **Matthieu Mottet**, *Quantum entanglement in carbon-carbon and carbon-homologues bonds*, Semester Student.

09.2011–01.2012 **Anna Hehn**, *Fock-space coupled cluster study of the halogen halides and halide dimers*, Master Student.

07.2010–10.2011 **Henk van Lingen**, *Electronic spectroscopy of the CUO molecule in noble gas matrices*, Master Student.

Teaching Experience

2013 **Quantum chemistry**, *ETH Zürich.*

2012 **Advanced physical chemistry**, *ETH Zürich.*

2010-2012 **C++ programming course for chemists**, *VU University Amsterdam.*

2009 **Quantum chemistry**, *VU University Amsterdam.*

Languages

Polish	**mother tongue**
English	**fluent**
Dutch	**communicative**
German	**basics**

Technical Experience

Extremely Proficient With

languages	Fortran 77/90, C/C++, Python
technologies	LaTeX, Git, Svn, Vim, Linux, OSX, Sphinx, ADF, Dirac, NWChem, Molpro, Horton, Dalton, Molcas, Gnuplot, MS/Open Office, Jmol, Avogadro, VESTA

Have Experience With

languages	Html, Turbo Pascal, Cshell
technologies	Windows, Turbomole, GAMESS (US), Gaussian, Molden, Molekel, Maxima, Mathcad, Statistica, Bash Scripting

Interests

Reading	Historical, scientific and bibliographical books
Movies	Action and science-fiction
Sport	Fitness, biking