Łukasz Mentel

Personal Information

Date of Birth	August 20, 1985	Place of Birth	Toruń, Poland
Nationality	Polish	Martial Status	Single

Education

2009 – 2014 **Ph.D. Studies in Theoretical Chemistry**, *Section Theoretical Chemistry*, Vrije Universiteit Amsterdam, The Netherlands.
http://www.chem.vu.nl

PH.D. THESIS

title *Reduced Density Matrix Inspired Approaches to Electronic Structure Theory*

supervisors Prof. E. J. Baerends and Dr. O. V. Gritsenko

available at https://dx.doi.org/10.6084/m9.figshare.1494690

2004 – 28.05.2009 **Master of Science in Chemistry**, *Department of Chemistry*, Nicolaus Copernicus University in Torun, Poland.
http://www.chem.uni.torun.pl

MASTER THESIS

title *Recovering four-component solutions by the inverse transformation of the infinite-order two-component (IOTC) wave functions*

supervisor Prof. Maria Barysz

Employment

2015 – **Postdoctoral Fellow**, *Catalysis Group*, Universitetet i Oslo, Norway.
http://www.mn.uio.no/ingap/english/

Exchange visits and collaborations

2010 – 2014 **Prof. K. S. Kim**, *Center for Superfunctional Materials*, Pohang University of Science and Technology (POSTECH), South Korea.
A total of two years were spent at POSTECH in seven visits thoughout four years

03.2016 – 06.2016 **Prof. J. Sauer**, *The Quantum Chemistry Research Group*, Humboldt-Universität zu Berlin, Germany.
https://www.chemie.hu-berlin.de/de/forschung/quantenchemie/standardseite

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Publications

1. O. V. Gritsenko, Ł. M. Mentel and E. J. Baerends. On the errors of local density (LDA) and generalized gradient (GGA) approximations to the Kohn-Sham potential and orbital energies. *J. Chem. Phys.*, **144**, no. 20, 204114 (2016).

2. D. Kędziera, Ł. Mentel, P. S. Żuchowski and S. Knoop. Ab initio interaction potentials and scattering lengths for ultracold mixtures of metastable helium and alkali-metal atoms. *Phys. Rev. A*, **91**, no. 6, 062711 (2015).

3. D. Kędziera and Ł. M. Mentel. Chasing the limits of the one electron approximation. In *AIP Conference Proceedings*, volume 1006, pages 1006–1008 (2014).

4. S. Knoop, P. Żuchowski, D. Kędziera, Ł. Mentel, M. Puchalski, H. P. Mishra, A. S. Flores and W. Vassen. Ultracold mixtures of metastable He and Rb: Scattering lengths from ab initio calculations and thermalization measurements. *Phys. Rev. A*, **90**, no. 2, 022709 (2014).

5. Ł. M. Mentel, R. van Meer, O. V. Gritsenko and E. J. Baerends. The density matrix functional approach to electron correlation: Dynamic and nondynamic correlation along the full dissociation coordinate. *J. Chem. Phys.*, **140**, no. 21, 214105 (2014).

6. Ł. Mentel and E. J. Baerends. Can the counterpoise correction for basis set superposition effect be justified? *J. Chem. Theory Comput.*, **10**, 252–267 (2014).

7. M. Borkowski, P. Żuchowski, R. Ciuryło, P. Julienne, D. Kędziera, Ł. Mentel, P. Tecmer, F. Münchow, C. Bruni and A. Görlitz. Scattering lengths in isotopologues of the RbYb system. *Phys. Rev. A*, **88**, no. 5, 052708 (2013).

8. Ł. Mentel, X. W. Sheng, O. Gritsenko and E. J. Baerends. On the formulation of a density matrix functional for Van der Waals interaction of like- and opposite-spin electrons in the helium dimer. *J. Chem. Phys.*, **137**, no. 20, 204117 (2012).

9. X. W. Sheng, Ł. Mentel, O. Gritsenko and E. J. Baerends. A natural orbital analysis of the long range behavior of chemical bonding and van der Waals interaction in singlet H2: The issue of zero natural orbital occupation numbers. *J. Chem. Phys.*, **138**, no. 16, 164105 (2013).

10. X. W. Sheng, Ł. Mentel, O. Gritsenko and E. J. Baerends. Counterpoise correction is not useful for short and Van der Waals distances but may be useful at long range. *J. Comput. Chem.*, **32**, no. 13, 2896–901 (2011).

11. M. Barysz, Ł. Mentel and J. Leszczyński. Recovering four-component solutions by the inverse transformation of the infinite-order two-component wave functions. *J. Chem. Phys.*, **130**, no. 16, 164114 (2009).

Computer Skills

OS All Microsoft™operating systems, Mac OS X™, Linux

Scripting bash, tcsh, csh, Perl, sed, Python 2.7.x/3.x, Numpy, Scipy, Pandas

Programming Fortran, 77/90/95/2003 standards

Tools Mathematica™, Octave, GNUPlot, Mercurial, SVN, Git

Office TEX, LATEX, Microsoft Office™, Open Office

Databases MongoDB, SQLite, PostgreSQL

www HTML, CSS, django, jekyll

Quantum chemistry packages

- ADF
- ASE
- DIRAC
- GAMESS US/UK/Atmol
- Gaussian
- Dalton
- MOLCAS
- NWChem
- Quantum Espresso
- SAPT
- TURBOMOLE
- VASP

Software

mendeleev Extensive database of atomic properties including 10 electronegativity scales, accessible via simple python API with powerful interactive visualization methods, more information at: http://mendeleev.readthedocs.io

chemtools A library of tools for manipulating one-electron basis sets including format conversions, optimization of exponents, visualization of completeness profiles, CBS extrapolations and more, available at: https://bitbucket.org/lukaszmentel/chemtools

batch calculator A GUI app for calculating the correct amounts of reactants (batch) for a particular composition given by the molar ratio of its components with a powerful database backend for storing and distributing the results: http://lmmentel.github.io/batchcalculator

panther Package for ANharmonic THERmochemistry - a python implementation for calculating anharmonic corrections to thermochemical functions in the independent mode approximation for molecules and solids, more information at: http://panther.readthedocs.io.

zefram A python interface for combined IZA and ZEOMICS databases of zeolite framework properties https://bitbucket.org/lukaszmentel/zefram.

bibler A convenience wrapper for BibTeX for automating bibliography handling https://bitbucket.org/lukaszmentel/bibler.

asetools A set of tools augmenting the functionality of ASE including a database schema for storing quantum chemical calculation results.

Contributed to

vconstr A suite of fortran programs primarily developed at the Section of Theoretical Chemistry at VU Amsterdam for reconstructing the exact Kohn-Sham potentials based on accurate densities https://bitbucket.org/lukaszmentel/vconstr.

ASE The Atomic Simulation Environment (ASE) is a set of tools and Python modules for setting up, manipulating, running, visualizing and analyzing atomistic simulations. https://wiki.fysik.dtu.dk/ase/

ase-espresso A Python interface for the Quantum Espresso code compatible with Atomic Simulation Environment (ASE) https://github.com/lmmentel/ase-espresso

Languages

English	fluent	Polish	fluent (mother tongue)
Dutch	basic	German	basic
Korean	basic		

Conferences and trainings

06 - 07.09.2016	Sigma2 HPC training seminar, Oslo, Norway
24 - 28.08.2015	Suncat Summer Institute - Heterogeneous Catalysis for Energy & Society, Stanford University, CA, USA
19.01-20.04.2015	Machine Learning Course by Andrew Ng, at Coursera.org, with an online certificate.
21 - 27.07.2014	EuroPython2014
10 - 11.02.2014	NWO CW Study Group Meeting, Chemistry in Relation to Physics and Materials Sciences, Velhoven, The Netherlands.
4 - 5.03.2013	NWO CW Study Group Meeting, Chemistry in Relation to Physics and Materials Sciences, Velhoven, The Netherlands.
17.11.2012	IV Symposium/Workshop of Computational Sciences, Pohang, Republic of Korea.
1 - 13.07.2012	12^{th} Sostrup Summer School in Quantum Chemistry and Molecular Properties, Himmelbjerget, Denmark.
12 - 16.12.2011	Winter School for Theoretical Chemistry and Spectroscopy, Han-sur-Lesse, Belgium.
17 - 22.07.2011	Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), Santiago de Compostela, Spain.
15 - 16.02.2010	Scientific meeting on Chemistry related to Physics & Material Sciences, Veldhoven, The Netherlands.
7 - 11.12.2009	Graduate Course on Theoretical Chemistry and Spectroscopy, Han-sur-Lesse, Belgium
21 - 22.11.2009	Symposium/Workshop of Computational Sciences, Pohang, Republic of Korea.
28.09 - 1.10.2008	7^{th} Central European Symposium on Theoretical Chemistry (CESTC 2008), Hejnice, Czech Republic.
9 - 13.06.2008	4^{th} Molcas Workshop, Bojnice, Slovakia.

Teaching Experience

2012	Preparing and conducting problem solving sessions and exams for *Molecular Quantum Mechanics* course at VU University.
2011	Preparing and conducting problem solving sessions and exams for *Theoretical Chemistry 1 & 2* course at VU University.
2010	Preparing and conducting problem solving sessions and exams for *Theoretical Chemistry 1 & 2* course at VU University.

Scientific Interests

- Electron Correlation
- Density Matrix Functional Theory
- Intermolecular Interactions
- Relativistic Quantum Chemistry
- Scientific computing, soft computing methods, fuzzy logic and cellular automata methods for numerical computation

Interests

Music playing trombone
Sports volleyball, football, hiking

References

VU University Amsterdam

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University of Oslo

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