PERSONAL INFORMATION

Family name, First name	Gori Giorgi, Paola
Date and place of birth	30 April 1971, Rome (Italy)
Nationality	Italian
E-mail	p.gorigiorgi.AT.vu.nl

EDUCATION

PhD

University	Department of Physics, University of Perugia (Italy)
Date of Award	14 February 2000
Supervisors	Prof. F. Sacchetti and Prof. G. B. Bachelet
Title of thesis	Electronic pair-distribution functions of jellium and real solids

Master ("Laurea")

University	Department of Physics, University of Rome "La Sapienza" (Italy)
Date of Award	29 February 1996
Supervisors	Prof. F. Melchiorri and Prof. F. A. Gianturco
Main subject	Cosmology and Astrochemistry
Title of thesis	Molecules in the early Universe
Final mark	110/110 <i>cum laude</i>

CURRENT POSITIONS

2016 -	Full Professor, Department of Theoretical Chemistry, VU University, Amsterdam
2009 - present	Tenured Senior Researcher (CR1), French National Research Council (CNRS),
-	Laboratoire de Chimie Théorique, Université Pierre et Marie Curie, Paris (France)
	[in temporary leave (détachement) since 2010]

PREVIOUS POSITIONS

2012 - 2015	Associate Professor, Department of Theoretical Chemistry, VU University, Amsterdam
2010 - 2012	Assistant Professor, Department of Theoretical Chemistry, VU University, Amsterdam
2005 - 2009	Tenured Junior Researcher (CR2), French National Research Council (CNRS),
	Laboratoire de Chimie Théorique, Université Pierre et Marie Curie, Paris (France)
2004	EU Marie Curie Fellow, Laboratoire de Chimie Théorique, Université Pierre et Marie
	Curie, (France)
2002 - 2003	Postdoctoral Fellow, Italian National Institute for Physics of Condensed Matter
	(INFM), Center for Statistical Mechanics and Complexity, Rome (Italy)
2001	Researcher, Department of Physics, University of Rome "La Sapienza" (Italy)
2000 - 2001	Postdoctoral Fellow, Department of Physics and Quantum Theory Group,
	Tulane University, New Orleans, Louisiana (USA)
1999 - 2000	Researcher, Department of Physics, University of Rome "La Sapienza" (Italy)
1996 – 1999	PhD Student, Department of Physics, University of Perugia (Italy)

FELLOWSHIPS AND AWARDS

- 2018 The Netherlands Organisation for Scientific Research (NWO) Innovational Research Incentives Scheme Vici (Talent scheme) *Disperion Interactions: A new theoretical approach in a pure density functional theory framework* (1.5M€)
- 2015 University Research Chair, Vrije Universiteit, Amsterdam, The Netherlands (75 K€)
- 2015 EU Horizon2020 **ERC Consolidator grant** *Improving the accuracy and reliability of electronic structure calculations: New exchange-correlation functionals from a rigorous expansion at infinite coupling strength* (2.0M€)
- 2011 The Netherlands Organisation for Scientific Research (NWO) Aspasia prize for excellent female academics (100K€)
- 2010 The Netherlands Organisation for Scientific Research (NWO) Innovational Research Incentives Scheme Vidi (Talent scheme) *Electronic density functional theory for strong-interacting systems* (800K€)
- 2004 Marie Curie Intra European Fellowship, From rigorous models to accurate energy density functionals (150 K€)
- 2000 Fellowship of the Italian Foundation "Angelo della Riccia" (15.3 K€)

VISITING SCIENTIST POSITIONS

- 2006 Quantum Theory Project, University of Florida (USA)
- 2002 Max Planck Institute for Physics of Complex Systems, Dresden (Germany)

ORGANIZATION OF INTERNATIONAL SCIENTIFIC CONFERENCES AND WORKSHOPS

- 2020 Organizer of the Faraday Discussion *New horizons in density functional theory*
- 2019 Organizer of the international workshop *Optimal Transport Methods in Density Functional Theory*, Banff International Research Station (BIRS), Canada
- 2017 Organizer of the international workshop *Optimal Transport meets Density Functional Theory*, Jyväskylä, Finland
- 2017 Organizer of the international conference *Promoting Female Excellence in Theoretical and Computational Chemistry*, Putten, The Netherlands
- 2015 Organizer of the international workshop *Advances in Electronic Structure Theory*, Jussieu Campus, Paris, France
- 2015 Organizer of the international conference *Computer Simulations for Condensed Phase Systems*, CNR Headquarters, Rome, Italy
- 2015 Organizer of the *Evert Jan Baerends Symposium*, VU University, Amsterdam, The Netherlands

INSTITUTIONAL RESPONSABILITIES

2012 – present	Member of the Works Council, Faculty of Exact Sciences,
-	VU University Amsterdam, The Netherlands
2012 - present	Organizer of the Amsterdam Center for Multiscale Modeling (ACMM) Symposia
	(see <u>http://www.acmm.nl/</u>)
2011 - 2014	Member of the Public Relation Committee, Department of Chemistry,
	VU University Amsterdam, The Netherlands

COMMISSIONS OF TRUST

2017 - 2018	Panel member START UP grant, Netherlands Organisation for Scientific Research (NWO)
2017	Member of the selection committee for the University Research Chair (VU, Amsterdam)
2015 and 2017	Panel member for the Vidi (Chemistry) grants committee, Netherlands Organisation for
	Scientific Research (NWO)
2014	Panel member for the ECHO (Excellent Chemical Research) grants committee,
	Netherlands Organisation for Scientific Research (NWO)
2014 - present	Member of several search committees for Assistant, Associate and Full Professor, VU

2014 - present Member of several search committees for Assistant, Associate and Full Profe University Amsterdam

MENTORING IN INTERNATIONAL PROGRAMS

2015 Mentor for the ProFiL-Programme (Technische Universität, the Humboldt Universität and the Freie Universität Berlin, Germany). ProFiL supports the career of the female researchers and prepares them for future leadership and management requirements of a professorship.

MEMBERSHIP OF INTERNATIONAL SCIENTIFIC BOARDS

- 2015 present DFT International Scientific Committee (organizing the International Conferences on Density-Functional Theory and its Applications)
- 2019 2020 Member of the International Advisory Board, Psi-k 2020 Conference

MEMBERSHIP OF NATIONAL SCIENTIFIC BOARDS AND RESEARCH CENTERS

- 2019 QuSoft: Research Center for Quantum Software
- 2019 Klankbordgroep Nationale Agenda Quantum Technologie
- 2010 Amsterdam Center for Multiscale Modeling (VU-UvA)

EDITORIAL ACTIVITIES

- 2021 Editorial Advisory Board Member, Journal of Physical Chemistry Letters (ACS)
- 2018 Editorial Board Member of *Electronic Structure (IOP Science)*
- 2016 Editor (with T. Helgaker, G. E. Scuseria, B. Silvi and J. Toulouse) of the *Special Issue in honour of Andreas Savin* in Molecular Physics (volume 114, issues 7-8).

SUPERVISION AND LEADERSHIP RESPONSABILITIES

2010 – present 1 UD, 9 Postdocs, 6 PhD Students Department of Theoretical Chemistry, VU University Amsterdam (The Netherlands)

MAJOR COLLABORATIONS

- E. J. Baerends (VU University, Amsterdam, The Netherlands): Fundamental aspects of KS DFT
- G. Buttazzo and L. De Pascale (Mathematics, University of Pisa, Italy): Optimal Transport and DFT
- S. Di Marino (Mathematics, Scuola Normale di Pisa, Italy): Optimal Transport and DFT
- A. Cohen and P. Mori-Sanchez (Chemistry, Cambridge and Madrid): Exact HK functional and SCE
- F. Della Sala and E. Fabiano (CNR Lecce, Italy): Benchmarking functionals based on SCE
- R. van Leeuwen (Physics, Jyväskylä University, Finland): time-dependent SCE
- M. Lewin (Matematics, CEREMADE, Paris Dauphine): jellium, Lieb-Oxford bound
- J. Lorenzana (Physics, University of Rome "La Sapienza", Italy): Lattice hamiltonians and DFT
- S. Moroni (SISSA, Trieste, Italy): Functionals for range-separated DFT from QMC
- Z. Musslimani (Mathematics, Florida State University, USA): SCE applied to disordered systems
- J. P. Perdew (Physics, Temple University, USA): Functionals from exact constraints and SCE
- E. Räsänen (Physics, Tempere University, Finland): Lieb-Oxford bound and SCE
- S. M. Reimann (Physics, Lund University, Sweden): SCE applications: quantum dots, cold atoms,...
- A. Rubio (Physics, Basque Country University, Spain): charge transfer with the SCE functional
- A. Savin (Chemistry, CNRS, University Paris VI, France): SCE and range separation
- A. Teale (Chemistry, Nottingham University, UK): exact quantities along the adiabatic connection
- C. J. Umrigar (Physics, Cornell University, USA): QMC results to benchmark SCE DFT
- C. Verdozzi (Physics, Lund University, Sweden): Green's functions and SCE
- G. Vignale (Physics, University of Missouri, USA): higher-order corrections to SCE

CAREER BREAKS

September 2010 – January 2011Maternity leave (6 months)January 2007 – June 2007Maternity leave (6 months)

SCIENTIFIC HIGHLIGHTS AND HONOURS

- 2018 Interviewed for the NWO ENW nieuwsbrief
- 2015 *University Research Chair* (VU Amsterdam). The URC is a selective and privileged appointment as full professor for excellent researchers
 - (www.vu.nl/en/research/topresearchers-at-vu/university-research-chair)
- 2015 Interviewed for *Elements*, the NWO annual magazine of chemical sciences.
- 2013 Chosen by the Netherlands Organisation for Scientific Research (NWO) for the vision document *Chemistry & Physics, Fundamental For Our Future.* The document describes the ambitions of the Netherlands for physics and chemistry for the next ten years and can be downloaded at www.nwo.nl/en/news-and-events/news/2013/cw/vision-document-chemistry-and-physics-in-2025-presented.html.
- 2012 Nominated by NWO for *AcademiaNet: Profiles of Leading Women Scientists* (www.academia-net.org)

POWER OF ATTRACTION TO YOUNG TALENTS

I have attracted very talented young researchers who have been awarded prestigious grants to work in my group: a Veni fellow (K. Giesbertz), and 4 Marie Curie IEF, of which three in Physics (F. Malet, G. Lani, Z. Musslimani) and one in Mathematics (A. Gerolin).

I have also had excellent PhD students among whom S. Vuckovic (cum laude) who has been awarded the Rubicon NWO grant to be a postdoctoral fellow at Irvine California (Burke group) and the Dick Stufkens prize for most outstanding PhD thesis of the Holland Research School of Molecular Chemistry.

SPOKEN LANGUAGES

Italian (mother tongue), English, French, Dutch

On-going Grants

Project Title	Funding Source	Amount	Period	Role
Dispersion Interactions: a new	The Netherlands			
theoretical approach in a pure	Organisation for			
Density Functional Theory	Scientific Research	1.5 M€	2019-2024	principal investigator
framework	(NWO) – Innovational			
	Research Incentives			
	Scheme Vici (Talent			
	scheme)			
Disordered and strongly-	EU – H2020 People			
correlated systems: a new	Marie Curie Intra	180 K€	2019-2021	host scientist in charge
theoretical approach	European Fellowship			
	Physics Panel			
	(Fellow: Prof. dr. Z.			
	Musslimani)			
Multi-marginal Optimal	EU – H2020 People			
Transport and Density	Marie Curie Intra	180 K€	2019-2021	host scientist in charge
Functional Theory: a	European Fellowship			
mathematical setting for	Mathematics Panel			
physical ideas	(Fellow: dr. A.			
	Gerolin)			

Previous Grants

Project Title	Funding Source	Amount	Period	Role
Improving the accuracy and reliability of electronic structure calculations: New exchange-correlation functionals from a rigorous expansion at infinite coupling strength	EU – Horizon2020 ERC Consolidator Grant Panel : PE4	2.0 M€	2015-2020	principal investigator
Strongly-correlated bosonic and fermionic ultracold atomic gases with long-range interactions: a new theoretical approach	Foundation for Fundamental Research on Matter (FOM) - Projectruimte	220 K€	2016-2019	principal investigator
The strictly-correlated- electrons approach at work for Chemistry: Density Functionals for transition metals and accurate excitation energies	The Netherlands Organisation for Scientific Research (NWO) - Free competition ECHO	260 K€	2013-2017	principal investigator
Time-dependent density functional theory for strongly- interacting electrons	EU – FP7 People Marie Curie Intra European Fellowship Physics Panel (Fellow: Dr. G. Lani)	180 K€	2014-2016	host scientist in charge
Strictly-correlated Density Functional Theory: methodology development and application to semiconductor nanostructures and ultracold atom gases	EU – FP7 People Marie Curie Intra European Fellowship Physics Panel (Fellow: Dr. F. Malet)	180 K€	2013-2015	host scientist in charge
Electronic density functional theory for strong-interacting systems	The Netherlands Organisation for Scientific Research (NWO) – Innovational Research Incentives Scheme Vidi (Talent scheme). Interdivisional panel	800 K€	2010-2015	principal investigator

INVITED TALKS (SELECTION) AT INTERNATIONAL CONFERENCES AND WORKSHOPS

I have been an invited speaker at about **50 international conferences** in the fields of Condensed Matter Physics, Quantum Chemistry and Mathematics. Here is a selection, divided by topic

Quantum and Theoretical Chemistry

- 2019 10th Congress of the International Society for Theoretical Chemical Physics, Tromso, Norway
- 2019 9th Molecular Quantum Mechanics, Heidelberg, Germany
- 2018 Satellite meeting to 16th ICQC: Strong correlation in electronic structure theory, Strasbourg, France
- 2018 16th International Congress of Quantum Chemistry, Menton, France
- 2017 57th Sanibel Symposium, St. Simons Island, Georgia, US
- 2014 Promoting Female Excellence in Theoretical and Computational Chemistry II, Oslo, Norway
- 2013 7th Molecular Quantum Mechanics, Lugano, Switzerland
- 2011 European Seminar on Computational Methods in Quantum Chemistry 2011, Oscarsborg, Norway
- 2009 92nd Canadian Chemistry Conference and Exhibition, Hamilton, Ontario, Canada
- 2008 6th Congress of the International Society for Theoretical Chemical Physics, Vancouver, BC, Canada
- 2007 16th Canadian Symposium on Theoretical Chemistry, St. John's, Newfoundland, Canada

Density Functional Theory in Electronic Structure

- 2019 CECAM Workshop: Improving the theory in DFT, Lausanne, Switzerland
- 2018 Adventures in Density Functional Theory and Beyond, ACS meeting, New Orleans, USA
- 2016 Symposium Recent Advances in Density Functional Theory and Applications in Chemical Physics, American Physical Society March Meeting, Baltimore, USA
- 2015 16th International Conference on Density Functional Theory and its Applications, Debrecen, Hungary
- 2015 Workshop on Fundamental Aspects of DFT, Oslo, Norway
- 2013 CECAM Workshop: Density Functional Theory: learning from the past, looking to the future, Berlin, Germany
- 2012 Challenges in Density Matrix and Density Functional Theory, Ghent, Belgium
- 2011 14th International Density Functional Theory (DFT) Conference, Athens, Greece
- 2011 *CECAM Workshop: How to speed up progress and reduce empiricism in Density Functional Theory*, Dublin, Ireland
- 2010 IX Girona Seminar: Electron Density, Density Matrices and Density Functional Theory, Girona, Spain
- 2006 Frontier Applications and Developments of Density Functional Theory, ACS Meeting, Atlanta, USA

Condensed Matter Theory; Electronic Structure in Physics; Many-body Physics

- 2017 Frontiers of Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond, Focus Session at the DPG Spring Meeting, Dresden, Germany
- 2017 18th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, Trieste, Italy
- 2016 7th Time-Dependent Density Functional Theory: Prospects and Applications, Benasque, Spain
- 2016 Condensed Matter Theory Division (European Physical Society) Topical Session on Theoretical spectroscopy: extending the ab-initio landscape, Groningen, The Netherlands
- 2015 Methods and Algorithms in Electronic Structure Theory, Ringberg Castle, Germany
- 2015 Psi-k 2015 Conference, San Sebastian, Spain
- 2013 CECAM Workshop: Green's functions Methods: the next generation, Toulouse, France
- 2014 *CECAM Workshop: What about U? Strong correlations from first principles,* Lausanne, Switzerland
- 2013 16th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, Trieste, Italy
- 2012 *Low-scaling and Unconventional Electronic Structure Techniques (LUEST) Conference*, Telluride Science Research Center, Colorado, USA
- 2011 Symposium on Many-electron approaches in Material Science; Mainz Materials Simulation Days 2011, Mainz, Germany
- 2006 30th International Workshop on Condensed Matter Theories, Dresden, Germany
- 2004 Third International Workshop on Electron Correlations and Materials Properties, Kos, Greece
- 2004 28th International Workshop on Condensed Matter Theories, St. Louis, USA

Optimal Transport, Mathematical Physics, Applied Mathematics

- 2019 Workshop Optimal Transport: from Geometry to Numerics, ESI, Vienna, Austria
- 2017 Applications of Optimal Transportation in the Natural Sciences, Oberwolfach, Germany
- 2016 *Putting the Theory Back in Density Functional Theory*, Institute for Pure and Applied Mathematics (IPAM) workshop and school, University of California, Los Angeles, USA
- 2015 New Trends in Optimal Transport, Bonn, Germany
- 2013 Semiclassical Origins of Density Functional Approximations, Institute for Pure and Applied Mathematics (IPAM) workshop, University of California, Los Angeles, USA
- 2013 Symposium "Electronic Structure" at Society for Industrial and Applied Mathematics (SIAM) Conference on Mathematical Aspects of Materials Science, Philadelphia, USA
- 2012 ERC Workshop on Optimal Transportation and Applications, Pisa, Italy

SCIENTIFIC PUBLICATIONS

[82] T.J. Daas, E. Fabiano, F. Della Sala, P. Gori-Giorgi, S. Vuckovic *Noncovalent interactions from models for the Møller-Plesset adiabatic connection* submitted to JPCL, arXiv:2104.04793

[81] T.J. Daas, J. Grossi, S. Vuckovic, Z.H. Musslimani, D.P. Kooi, M. Seidl, K.J.H. Giesbertz, P. Gori-Giorgi Large coupling-strength expansion of the Møller-Plesset adiabatic connection: From paradigmatic cases to variational expressions for the leading terms J. Chem. Phys. 153, 214112 (2020)

[80] D. P. Kooi and P. Gori-Giorgi London dispersion forces without density distortion: a path to first principles inclusion in density functional theory Faraday Discussions 224, 145 (2020)

[79] J. Grossi, Z. H. Musslimani, M. Seidl, P. Gori-Giorgi Kohn-Sham equations with functionals from the strictly-correlated regime: Investigation with a spectral renormalization method J. Phys.: Cond. Matt. 32 475602 (2020)

[78] D. P. Kooi, T. Weckman, P. Gori-Giorgi*Dispersion without many-body density distortion: Assessment on atoms and small molecules*J. Chem. Theory Comput., 17, 2283 (2021)

[77] S. Vuckovic, E. Fabiano, P. Gori-Giorgi, K. Burke *MAP: an MP2 accuracy predictor for weak interactions from adiabatic connection theory* J. Chem. Theory Comput. 16, 4141 (2020)

[76] A. Gerolin, J. Grossi, P. Gori-Giorgi *Kinetic correlation functionals from the entropic regularisation of the strictly-correlated electrons problem* J. Chem. Theory Comput. 16, 488 (2020)

[75] S. Giarrusso, P. Gori-Giorgi Exchange-Correlation Energy Densities and Response Potentials: Connection Between Two Definitions and Analytical Model for the Strong-Coupling Limit of a Stretched Bond J. Phys. Chem. A 124, 2473 (2020)

[74] J. Grossi, M. Seidl, P. Gori-Giorgi, K.J.H. Giesbertz Functional Derivative of the Zero Point Energy Functional from the Strong Interaction Limit of Density Functional Theory Phys. Rev. A 99, 052504 (2019)

[73] D. P. Kooi, P. Gori-Giorgi *A variational approach to London dispersion interactions without density distortion* J. Phys. Chem. Lett. 10, 1537 (2019)

[72] E. Fabiano, S. Śmiga, S. Giarrusso, T. J. Daas, F. Della Sala, I. Grabowski, P. Gori-Giorgi Investigation of the exchange-correlation potential of functionals based on the adiabatic connection interpolation

J. Chem. Theory Comput. 15, 1006 (2019)

[71] M. Seidl, S. Giarrusso, S. Vuckovic, E. Fabiano, P. Gori-Giorgi Strong-interaction limit of an adiabatic connection in Hartree-Fock theory J. Chem. Phys. 149, 241101 (2018) (Communication)

[70] D. P. Kooi and P. Gori-Giorgi

Local and global interpolations along the adiabatic connection of DFT: A study at different correlation regimes

Theor. Chem. Acc. 137, 166 (2018) (special issue Ad Memoriam Janos Angyan)

[69] S. Giarrusso, S. Vuckovic, P. Gori-Giorgi Response potential in the strong-interaction limit of DFT: Analysis and comparison with the coupling-constant average J. Chem. Theory Comput., 14, 4151 (2018)

[68] S. Giarrusso, P. Gori-Giorgi and K. J. H. Giesbertz Sum-rules of the response potential in the strongly-interacting limit of DFT Eur. Phys. J. B 91, 186 (2018) (special issue in honour of E.K.U. Gross)

[67] P. Gori-Giorgi and E. J. Baerends Asymptotic nodal planes in the electron density and the potential in the effective equation for the square root of the density

Eur. Phys. J. B 91, 160 (2018) (special issue in honour of E.K.U. Gross)

[66] S. Vuckovic, P. Gori-Giorgi, F. Della Sala, E. Fabiano Restoring size consistency of approximate functionals constructed from the adiabatic connection J. Phys. Chem. Lett. 9, 3137 (2018).

[65] S. Giarrusso, P. Gori-Giorgi, F. Della Sala, E. Fabiano Assessment of interaction-strength interpolation formulas for gold and silver clusters J. Chem. Phys. 148, 134106 (2018).

[64] S. Vuckovic, M. Levy, and P. Gori-Giorgi Augmented potential, energy densities, and virial relations in the weak- and strong-interaction limits of DFT J. Chem. Phys. 147, 214107 (2017). Featured Article; Editor's Choice

[63] J. Grossi, D. P. Kooi, K. J. H. Giesbertz, M. Seidl, A. J. Cohen, P. Mori-Sanchez, P. Gori-Giorgi Fermionic statistics in the strongly correlated limit of Density Functional Theory J. Chem. Theory Comput. 13, 6089 (2017)

[62] S. Vuckovic and P. Gori-Giorgi Simple fully non-local density functionals for the electronic repulsion energy J. Phys. Chem. Lett. 8, 2799 (2017); highlighted in *Spotlights*

[61] M. Seidl, S. di Marino, A. Gerolin, L. Nenna, K.J.H. Giesbertz, and P. Gori-Giorgi The strictly-correlated electron functional for spherically symmetric systems revisited Phys. Rev. A, submitted (arXiv:1702.05022), needs to be revised and split in two articles

[60] S. Vuckovic, T.J.P. Irons, L.O. Wagner, A.M. Teale, and P. Gori-Giorgi Interpolated energy densities, correlation indicators and lower bounds from approximations to the strong coupling limit of DFT Phys. Chem. Chem. Phys. 19, 6169 (2017)

[59] E. Fabiano, P. Gori-Giorgi, M. Seidl and F. Della Sala Interaction-Strength Interpolation Method for Main-Group Chemistry: Benchmarking, Limitations, and Perspectives
J. Chem. Theory Comput. 12, 4885 (2016)

[58] S. Vuckovic, T.J.P. Irons, A. Savin, A.M. Teale, and P. Gori-Giorgi *Exchange-correlation functionals via local interpolation along the adiabatic connection* J. Chem. Theory Comput. 12, 2598 (2016) (ACS Editor's choice)

[57] G. Lani, S. di Marino, A. Gerolin, R. van Leeuwen, and P. Gori-Giorgi *The adiabatic strictly-correlated electron functional: kernel and exact properties* Phys. Chem. Chem. Phys., 18, 21092 (2016)

[56] Z.-J. Ying, V. Brosco, G. M. Lopez, D. Varsano, P. Gori-Giorgi, and J. Lorenzana Anomalous scaling and breakdown of conventional density functional theory methods for the description of Mott phenomena and stretched bonds Phys. Rev. B 94, 075154 (2016)

[55] M. Seidl, S. Vuckovic, and P. Gori-Giorgi *Challenging the Lieb-Oxford bound in a systematic way* Mol. Phys. 114, 1076 (2016)

[54] P. Gori-Giorgi, T. Gal, and E. J. Baerends Asymptotic behavior of the electron density and the Kohn-Sham potential in case of a Kohn-Sham HOMO nodal plane Mol. Phys. 114, 1086 (2016)

[53] F. Malet, A. Mirtschink, C. B. Mendl, J. Bjerlin, E. O. Karabulut, S. M. Reimann, and P. Gori-Giorgi *Density functional theory for strongly-correlated bosonic and fermionic ultracold dipolar and ionic gases* Phys. Rev. Lett., 115, 033006 (2015) (Editor's suggestion)

[52] S. Vuckovic, L. O. Wagner, A. Mirtschink, and P. Gori-Giorgi *Hydrogen molecule dissociation curve with functionals based on the strictly-correlated regime* J. Chem. Theory Comput. 11, 3153 (2015)

[51] L. O. Wagner and P. Gori-Giorgi *Electron avoidance: A nonlocal radius for strong correlation* Phys. Rev. A 90, 052512 (2014)

Phys. Rev. B 89, 125106 (2014)

[50] F. Malet, A. Mirtschink, K. J. H. Giesbertz, L. O. Wagner, and P. Gori-Giorgi *Exchange-correlation functionals from the strongly-interacting limit of DFT: Applications to model chemical systems* Phys. Chem. Chem. Phys. 16, 14551 (2014)

[49] A. Mirtschink, C. J. Umrigar, J. D. Morgan III, and P. Gori-Giorgi *Energy Density Functionals From the Strong-Coupling Limit Applied to the Anions of the He Isoelectronic Series*J. Chem. Phys. 140, 18A532 (2014) (invited article)

[48] C. B. Mendl, F. Malet, and P. Gori-Giorgi Wigner localization in quantum dots from Kohn-Sham density functional theory without symmetry breaking

[47] F. Malet, A. Mirtschink, K. J. H. Giesbertz, and P. Gori-Giorgi Density Functional Theory for strongly-interacting electrons in "Many-Electron Approaches in Physics, Chemistry and Mathematics: A Multidisciplinary View", Springer Verlag 2014, Book Series: Studies in Mathematical Physics, edited by L. Delle Site and V. Bach. [46] A. Mirtschink, M. Seidl, and P. Gori-Giorgi Derivative discontinuity in the strong-interaction limit of density functional theory Phys. Rev. Lett. 111, 126402 (2013)

[45] F. Malet, A. Mirtschink, J. C. Cremon, S. M. Reimann, and P. Gori-Giorgi *Kohn-Sham density functional theory for quantum wires in arbitrary correlation regimes* Phys. Rev. B 87, 115146 (2013) (Editor's suggestion)

[44] F. Malet and P. Gori-Giorgi *Strong correlation in Kohn-Sham density functional theory* Phys. Rev. Lett. 109, 246402 (2012)

[43] A. Mirtschink, M. Seidl, and P. Gori-Giorgi*Energy densities in the strong-interaction limit of density functional theory*J. Chem. Theory Comput. 8, 3097 (2012)

[42] G. Buttazzo, L. De Pascale, and P. Gori-Giorgi *Optimal-transport formulation of electronic density-functional theory* Phys. Rev. A 85, 062502 (2012)

[41] E. Räsänen, M. Seidl, and P. Gori-Giorgi *Strictly correlated uniform electron droplets* Phys. Rev. B 83, 195111 (2011)

[40] P. Gori-Giorgi and M. Seidl Density functional theory for strongly-interacting electrons: Perspectives for Physics and Chemistry Phys. Chem. Chem. Phys. 12, 14405 (2010) (invited article)

[39] M. Seidl and P. Gori-Giorgi *Adiabatic connection at negative coupling strengths* Phys. Rev. A 81, 012508 (2010)

[38] P. Gori-Giorgi, M. Seidl, and G. Vignale Density functional theory for strongly interacting electrons Phys. Rev. Lett., 103, 166402 (2009) (highlighted with a **Synopsis in** *Physics* and as **Editor's suggestion**)

[37] P. Gori-Giorgi, J. G. Angyan, and A. Savin *Charge density reconstitution from approximate exchange-correlation holes* Can. J. Chem. 87, 1444 (2009) (invited article)

[36] P. Gori-Giorgi, G. Vignale, and M. Seidl *Electronic zero-point oscillations in the strong-interaction limit of density functional theory* J. Chem. Theory Comput. 5, 743 (2009)

[35] P. Gori-Giorgi and A. Savin Study of the discontinuity of the exchange-correlation potential in an exactly soluble case Int. J. Quantum Chem. 109, 2410 (2009) (invited article)

[34] P. Gori-Giorgi and A. Savin Range separation combined with the Overhauser model: Application to the H₂ molecule along the dissociation curve Int. J. Quantum Chem. 109, 1950 (2009) (invited article)

[33] P. Gori-Giorgi, M. Seidl and A. Savin Intracule densities in the strong-interaction limit of density functional theory Phys. Chem. Chem. Phys. 10, 3440 (2008) (invited article) [32] P. Gori-Giorgi and A. Savin Degeneracy and size consistency in electronic density functional theory J. Phys.: Conf. Ser. 117, 012017 (2008) (invited article)

[31] P. Gori-Giorgi and A. Savin *The high-density limit of two-electron systems: Results from the extended Overhauser approach* J. Chem. Theory Comput. 3, 796 (2007)

[30] M. Seidl, P. Gori-Giorgi, and A. Savin Strictly correlated electrons in density functional theory: A general formulation with applications to spherical densities Phys. Rev. A 75, 042511 (2007)

[29] P. Gori-Giorgi and A. Savin *Kohn-Sham calculations combined with an average pair-density functional theory* Int. J. Mod. Phys. B 21, 2449 (2007) (invited article)

[28] P. Gori-Giorgi, J. Toulouse, and A. Savin Model hamiltonians in density functional theory in "High-dimensional Partial Differential Equations in Science and Engineering", CRM Proceedings & Lecture Notes 41, 117 (2007) (invited contribution)

[27] E. Goll, H.-J. Werner, H. Stoll, T. Leininger, P. Gori-Giorgi, and A. Savin A short-range gradient-corrected spin density functional in combination with long-range coupled-cluster methods: Application to alkali-metal rare-gas dimers Chem. Phys. 329, 276 (2006)

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OTHER PUBLICATIONS

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OTHER: INTERVIEWS IN THE DUTCH MEDIA ON THE PROBLEMS OF HIGHER EDUCATION

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Waarom hoogleraren en docenten vandaag een rood vierkantje dragen, NOS September 2018 <u>https://nos.nl/op3/artikel/2248796-waarom-hoogleraren-en-docenten-vandaag-een-rood-vierkantje-dragen.html</u>

TEACHING ACTIVITIES

2011 Dutch University Teaching Certification (BKO)

Mathematics in the Bachelor Chemistry (joint degree UvA-VU)

Since 2014 I have played a key role in redesigning, coordinating and teaching the mathematics of this joint degree. In particular, I have been asked to design a new compulsory course:

- Wiskunde voor Chemici III (3EC) 2018 – present [coordinator and lecturer]

2nd year Bachelor Chemistry (joint degree UvA-VU): basic mathematics needed for quantum mechanics. This course has solved the long-standing difficulties of chemistry students with quantum mechanics and had very positive evaluations already in the first year I have taught it.

The course Wiskunde II, which the students follow in the 1st year, is since 2017 taught by dr. K. Giesbertz, UD in our group. This way, we carefully design together the two courses. On top of that, I have been teaching for several years an elective course

- Mathematics for Quantum Chemistry (6EC) 2014 – present [coordinator and lecturer] 3rd year Bachelor Chemistry (joint degree UvA-VU): more advanced mathematical aspects of quantum chemistry.

Concept:

What made the students appreciate these Mathematics courses is both their content (carefully selected to cover the material they really need for quantum and physical chemistry, with several examples that connect concepts they have seen in previous courses with their mathematical aspects) and the methodology of teaching that I have designed. Each topic is treated in the following way:

- Explanation at the blackboard for 15-20 minutes
- Distribution of handouts containing
 - Key equations/concepts I have just explained
 - An exercise to do immediately
 - o While they do the exercise, I walk in the class to identify problems/points that remained unclear
 - Back at the blackboard I address the problems and the unclear points I have observed
- Explain the next topic in the same way

Exercise classes are also scheduled, where more difficult exercises are treated. For the elective course I also use assignments that they have to hand in. This helps the students to keep the right pace during the course.

During the pandemic, I have switched to video clips for each topic. The videos have received extremely good evaluations from the students, and I will re-use them in a blended learning approach in future years.

Basic Physics in other programs

Since 2014, I have been coordinating and teaching basic physics courses in various programs at the VU. These courses are challenging because the students are not very interested in the subject. I have been experimenting with different ways to capture their interest, in particular by linking the concepts to the main topic of their studies and by using several online self-study platforms.

- Natuurkunde & Wiskunde voor Chemici I (6 EC) 2010 2012 [coordinator and lecturer] 1st year Bachelor Chemistry: calculus and classical mechanics combined
- BasisNatuurkunde (3EC) 2015 2018 [coordinator and lecturer]
- st year Bachelor Pharmaceutical Sciences: elements of classical mechanics and electromagnetism
 Fysica 1: Mechanica (3EC) 2018 present [coordinator and lecturer]
 - 1st year Bachelor Science, Business and Innovation: elements of classical mechanics
 - Fysica 1: Mechanica (3EC) 2018 present [coordinator and lecturer]
 - 1st year Bachelor Medische Natuurwetenschappen: elements of classical mechanics

During the pandemic, I have used video clips where I carefully explain each topic and where I solve step by step sample exercises.

Quantum Mechanics in the Bachelor and Master Chemistry

I have been involved as lecturer in various Quantum Mechanics/Quantum Chemistry courses in both the Bachelor and the Master Chemistry. In the students' evaluations I have been always appreciated for my clear explanations of concepts that are very difficult for them. I have used also in these courses the same methodology of my Mathematics courses, combining explanations at the blackboard with handouts.

- Theoretische Chemie 1 & 2 (6 EC): 2011 [lecturer with L. Visscher]
- 2nd year Bachelor Chemistry: introductory quantum mechanics and applications to atoms and molecules
 Moleculaire Quantummechanica (6EC): 2012 [lecturer with L. Visscher]
- 2nd year Bachelor Chemistry: introductory quantum mechanics and applications to atoms and molecules
 Quantum Theory of Molecules and Matter (6EC): 2014 2018 [lecturer with W.J. Buma & H. Zhang]
- 1st year Master Chemistry: quantum mechanics and applications from atoms to solids
- Understanding Quantum Chemistry (6EC): 2018 [lecturer with L. Visscher]
 1st year Master Chemistry: methods in quantum chemistry: Hartree-Fock, DFT, coupled clusters

Other lectures and courses in Physics programs

2001	Exercise classes Quantum Mechanics for Physics undergraduates, Tulane University, US
2002 - 2004	Lecturer for Solid State and Molecular Physics in the master ("Laurea") program in
	Physics – University of Rome "La Sapienza" (Italy)
2019	Guest lecturer (1 lecture on DFT) for the course Advanced numerical methods in many-
	body physics, Master Physics & Astronomy UvA (coordinator and lecturer: P. Corbez).

Lecturer in International Advanced Schools:

2017	Virtual Winter School on Computational Chemistry (https://winterschool.cc/)
2016	Lecturer at the school Putting the theory back in Density Functional Theory, IPAM,
	Los Angeles (USA)
2013	Lecturer at the doctorate Han-sur-Lesse Winter School in Theoretical Chemistry and
	Spectroscopy (Belgium)

Supervision of Bachelor and Master Projects

I have supervised several bachelor and master projects in Chemistry, Mathematics and Physics.

PhD juries

2008 – present Opponent in more than 30 PhD defenses in the Netherlands, Europe, and US