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@vu.nl

EDUCATION

PhD in Physics

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 ***cum laude***

CURRENT POSITIONS

2022 –	Principal Research Manager, Microsoft Research AI4Science, Amsterdam
2016 –	Professor (full) of Theoretical and Mathematical Chemistry, VU University, Amsterdam
2009 –	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** (highly selective talent scheme, 10-15% success rate) *Dispersion 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 European Research Council (**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** (highly selective talent scheme, 10-15% success rate) *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€)

SCIENTIFIC HIGHLIGHTS AND HONOURS

2018 Interviewed for the Netherlands Organization for Scientific Research (NWO) news

2017 - *University Research Fellowship* (VU Amsterdam). Talented Bachelor and Master students can apply for the University Research Fellowship (URF) which carries my name. The URF is a token of appreciation to the university's most excellent scientists for their extraordinary research performances.

2016 - *University Research Chair* (VU Amsterdam). The URC is a selective and privileged appointment as full professor for excellent researchers

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.

2012 Nominated by NWO for *AcademiaNet: Profiles of Leading Women Scientists*

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 Committee 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 – 2019 Organizer of the Amsterdam Center for Multiscale Modeling (ACMM) Symposia (see http://www.acmm.nl/)

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 University Amsterdam and other Dutch Universities

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

EDITORIAL ACTIVITIES

2021 - Editorial Advisory Board Member, *Journal of Physical Chemistry Letters* (ACS)
2018 - 2022 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, LEADERSHIP RESPONSABILITIES AND MENTORING

Since 2010 I have been leading the research group *Quantum Matter in Chemistry & Physics* located at the Theoretical Chemistry division of VU Amsterdam.
The average size of the group during the years varied between 5-10 members. I was responsible for selecting the group members, guiding them in their research projects, mentoring and coaching them, and helping them transitioning to their next position. More precisely, I have been supervising:

1 Assistant Professor (tenured position in the NL)
9 Postdocs
8 PhD Students
1 Technician (computer administrator)
4 young fellows under the University Research Fellowship of the VU Amsterdam

All my former PhD students have completed their PhD within the expected 4 years, and they all had excellent postdoctoral offers in leading groups of Computational & Theoretical Chemistry. On going PhD students are also perfectly on track.

Several of my mentees have very successful careers in academia (e.g., Stefan Vuckovic, lecturer at the University of Bristol, who was awarded several prestigious grants; Augusto Gerolin, Assistant Professor and Canadian Research Chair at the University of Ottawa; Hilke Bahmann, Emmy Noether junior group leader at the University of Saarland), in industry (e.g., Lucas Wagner, software engineer at Google; Francesc Malet, modeling analyst at ABN AMRO), and also in creating their own start up with the support of my network within the VU demonstrator lab (e.g., Mehdi Farzanehpour, founder and CEO of SciToDate).

Supervision of Bachelor and Master Projects

I have supervised > 30 bachelor and master projects in Chemistry, Mathematics and Physics.

PhD juries

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

POWER OF ATTRACTION TO YOUNG TALENTS

I have attracted very talented young researchers who have been awarded prestigious grants: 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 such as 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.

FOSTERING DIVERSITY IN ACADEMIA

I have been a 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.

In 2017 I organized (with Ria Broer, Celia Fonseca Guerra and Jocelyne Vreede) the international conference *Promoting Female Excellence in Theoretical and Computational Chemistry*. The format is designed to create the reverse situation in usual conferences, with 70% of female (or other) speakers and 30% of male speakers. It is part of a series of conferences that showcase and raise awareness on excellence in the field besides the usual represented groups.

COMMITMENT FOR A BETTER ACADEMIA

I am in the core group of WOinActie, as contact point for the VU Amsterdam.
WOinActie is a Dutch movement uniting academics, students and university boards to demand the government to provide proper funding for research and education. I have been interviewed in Dutch media several times on the issues that particularly young people face within the Dutch academia, and I have co-authored a position paper with a vision to move forward.
As WOinActie@VU contact point, I have contributed to unite academics from very different disciplines, creating a strong network inside the university, overcoming several differences and communication problems within different fields. In the WOinActie core group, I have worked together with people from all over the Netherlands in all the different disciplines.

2021: Speaker/Panelist at Caring for Science, organized by the Amsterdam Young Academy.

I have written articles on the problems of social safety/harassment and alike in academia, and I have been interviewed on the issues by the Royal Academy of Science committee on social safety in Dutch academia.

MAJOR SCIENTIFIC 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 2011	Maternity leave (6 months)
January 2007 – June 2007	Maternity leave (6 months)

SPOKEN LANGUAGES

Italian (mother tongue), English, French, Dutch

TEACHING ACTIVITIES

2011 Dutch University Teaching Certification (BKO)

Mathematics in the Bachelor Chemistry (joint degree University of Amsterdam-VU)

Since 2014 I have played a key role in redesigning, coordinating and teaching the whole mathematics of this joint degree. Moreover, I have designed and taught 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.

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.

Basic Physics in other programs

Since 2014, I have been coordinating and teaching basic physics courses in various programs at the VU:

- 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]
  1st 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

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.

- 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)

Recent and Ongoing Grants

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

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 **60 international conferences** in the fields of Condensed Matter Physics, Quantum Chemistry and Mathematics. Here is a selection, divided by topic

Quantum and Theoretical Chemistry

2021 *CECAM Workshop: Non-Covalent Interactions in Large Molecules and Extended Materials*, Lausanne, Switzerland
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

2022 *Psi-k Conference, Lausanne*
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

2021 *CECAM Workshop: Recent developments in quantum Monte Carlo*, Rome, Italy
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
2022 *Workshop: Model Reduction in Quantum Mechanics*, IPAM [talk online]
2021 *Society for Industrial and Applied Mathematics (SIAM) Conference on Mathematical Aspects of Materials Science*, online
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

See full list with pdf files at https://quantummatter.eu/publications

Google Scholar profile: https://scholar.google.com/citations?user=9ZZbdlIAAAAJ&hl=en