Leonardo Guidoni – Curriculum Vitae

Personal Data

Name	Leonardo Guidoni
Place, date of birth	Roma (Italy), Jan 8th, 1972
Citizenship	Italian
Marital status	Married
Current Position	Full Professor in Chemical Phisics 03/A2 CHIM/02
Qualification	National Scientific Qualification as Full Professor: 03/B1, 03/B2, 02/B2, 02/D1
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Education, Fellowships and Positions

Jan 2021-	Full Professor of Physical Chemistry at the University of L'Aquila
Dec 2008-2020	Associate Professor in Chemistry at the University of L'Aquila
Jan 2007	Qualification to University Professor in France ("Qualification au Professeur des universités")
Aug-Sep 2006	Invited Professor at the University of Leiden, The Netherlands.
Aug-Sep 2005	Invited Professor at the Swiss Federal Institute of Technology in Lausanne, Switzerland.
2004-2008	"Brain Gain" Professorship (Professore a Contratto "Rientro Cervelli") in Computational Biophysics and Biochemistry at the department of Physics of the University of Rome "La Sapienza".
Jul 2002	Post-doctoral position at the Swiss Federal Institute of Technology in Lausanne, Institute of Molecular Chemistry and Biology, in the group of Prof. U. Röthlisberger.
Nov 2000	Post-doctoral position at the Swiss Federal Instutute of Technology in Zürich, Department of Inorganic Chemistry, in the group of Prof. U. Röthlisberger.
Oct 2000	Doctor Philisophiæ degree *cum laude* in Theory of Condensed Matter at the International School for Advanced Studies of Trieste. Thesis: *Theoretical Studies on the KcsA Potassium Channel.* Supervisors: P. Carloni, V.Torre.
1997	Civilian service.
Jul 1996	Degree in Physics at Università degli Studi di Roma "La Sapienza" with first class honors (mark 110/110 *cum laude*). Thesis: *Spin system with orbital degeneracy: lattice Quantum Monte Carlo.* Supervisors: G.B. Bachelet, G. Santoro, S. Sorella.

Languages Italian (mother tongue), English (fluent)

Teaching activity

All the following course are intended as full courses, if not differently specified.

For the *Bachelor in Biotechnology* at the University of L'Aquila

Oct/Jan 2017	"General Chemistry"
Oct/Jan 2016	"General Chemistry"
Oct/Jan 2015	"General Chemistry"
Oct/Jan 2014	"General Chemistry"
Oct/Jan 2012	"General Chemistry"

For the *Bachelor in Engineering* at the University of L'Aquila
Feb/May 2020 "General Chemistry"
Feb/May 2019 "General Chemistry"
Mar/May 2018 "General Chemistry"
Mar/May 2011 "General Chemistry"
Mar/May 2010 "General Chemistry"
Mar/May 2009 "General Chemistry"

For the *Bachelor in Chemistry* at the University of L'Aquila
Feb/May 2020 "Stoichiometry and Laboratory of Chemistry" (shared course)
Mar/May 2018 "Stoichiometry and Laboratory of Chemistry" (shared course)

For the *Master in Chemistry* at the University of L'Aquila
Oct/Jan 2022 "Physical Chemistry II"
Oct/Jan 2022 "Theoretical Chemistry"
Oct/Jan 2021 "Physical Chemistry II"
Oct/Jan 2021 "Theoretical Chemistry"
Feb/May 2020 "Theoretical Chemistry"
Feb/May 2019 "Computer Modelling and Simulations of Biomolecules"
Oct/Jan 2017 "Computer Modelling and Simulations of Biomolecules"

For the *Master in Chemistry and the Master in Mathematical Engineering* at the University of L'Aquila
Oct/Jan 2016 "Computer Modelling and Simulations of Biomolecules"
Oct/Jan 2015 "Computer Modelling and Simulations of Biological Systems"
Oct/Jan 2014 "Computer Modelling and Simulations of Biological Systems"

For the *Master in Mathematical Engineering* at the University of L'Aquila
Oct/Jan 2012 "Computer Modelling and Simulations of Biological Systems"
Oct/Jan 2012 "Principles of Structural and Cell Biochemistry"
Oct/Jan 2011 "Computer Modelling and Simulations of Biological Systems"
Oct/Jan 2011 "Principles of Structural and Cell Biochemistry"
Oct/Jan 2010 "Computer Modelling and Simulations of Biological Systems"
Oct/Jan 2010 "Principles of Structural and Cell Biochemistry"
Mar/May 2009 "Computer Modelling and Simulations of Biological Systems"

For the *PhD in Mathematical Engineering and the PhD in Informatics* at the University of L'Aquila
Jan 2020 "Introduction to Quantum Computing" (6 hours)

For the *PhD in Mathematical Engineering and the PhD in Physics and Chemistry* at the University of L'Aquila
Dec 2018 "Introduction to Quantum Computing" (4 hours)

For the *Bachelor in Physics* at the University of Rome "La Sapienza"
Apr/Jun 2007 "Mechanics of Material Point" (esercitazioni)
Jan/Mar 2007 "General Mechanics" (esercitazioni)
Apr/Jun 2006 "Mechanics of Material Point" (esercitazioni)
Jan/Mar 2006 "General Mechanics" (esercitazioni)

For the *Master in Physics* at the University of Rome "La Sapienza"
Oct 2007-Dec 2007 "Atomistic Simulation" (full course)
Oct 2006-Dec 2006 "Atomistic Simulation" (full course)
Oct 2005-Dec 2005 "Atomistic Simulation" (full course)

For the *Phd in Physics* at the University of Rome "La Sapienza"
Mar/May 2007 "Theoretical Physics of Condensed Matter" (about 20 hours)

Mar/May 2006 "Theoretical Physics of Condensed Matter" (about 20 hours)
Mar 2005-May 2005 "Molecular Dynamics" (about 20 hours)

For the *Bachelor in Chemistry* at the École Polytechnique Fédérale de Lausanne
2002-2004 "Computational Chemistry" (assistant)
2002-2004 "General Chemistry" (assistant)

Supervisor Experience

LG supervised several *Bachelor, Master and PhD Students* in *Chemistry, Biochemistry, Physics, Biophysics, Material Science and Mathematical Engineering* curricula at University of L'Aquila, at Sapienza Università di Roma, and at Università di Roma3.
The subjects of the majority of the PhD and Bachelor Theses are Theoretical Chemistry Computational Biochemistry and Molecular Modelling, Quantum Chemistry and Theoretical Chemical Physics. The SSD assigned to PhD theses are different: CHIM/02, CHIM/07 and FIS/03.

Supervised PhD Students: Leonardo Ratini, Chiara Capecci, Cintia Scafa Urbaez Vilchez, Mario Frezzini, Daniele Ottaviani, Fabio Pitari, Matteo Capone, Giovanna Rogati, Francesco Cappelluti, Aliya Tichengulova, Barbara Gregori, Godfred Epie Essongolle, Daniele Bovi, Matteo Barborini, Gaia Di Paolo, Maria Montagna.

Supervised Master Students: Francesco Amori, Gianluca Parisse, Noemi di Stefano, Leonardo Serilli, Chiara Capecci, Yahya Saleh, Mario Frezzini, Eduard Elias, Fabio Pitari, Marco Alfieri, Barbara Gregori, Daniele Bovi, Henry Martin, Diego Di Girolamo, Andrea Di Luca, Pietro De Gaetano, Luana Tanzi, Chiara Pasquini, Caterina De Franco, Marco Manzoli, Ganesh Sivaraman, Kwame Atta Gyamfi, Eleonora Amici, Miriam Garcia-Soto, Marco Magliocchetti, Delyan Zelyazov, Olga Chernomor, Magdalena Szçzesna, Gaia Di Paolo, Maria Montagna, Alessandro Lovato.

Supervised Bachelor Students: Andrea Pagliarini, Davide Ubaldi, Davide Fontana, Chiara Capecci, Davide Sabeddu, Silvia Menghi, Mohammad Nurul Islam, Paola Malacari, Michela Ronti, Jared Lolli, Marco Alfieri, Fabio De Vellis.

Supervised Post-docs: Daniele Narzi, Daniele Varsano, Emanuele Coccia, Andrea Zen, Daniele Bovi, Francesco Benfenati, Shin Nakamura, Chao Zhang, Antonio Di Martino, Andrea Zen, Fabio Sterpone.

Supervised graduate fellows:
Matteo Capone, Cintia Scafa, Andrea Di Stefano, Miriam Garcia Soto.

LG was also committed as external referee for several PhD theses (University of Helsinki, SISSA-Trieste, Università di Roma La Sapienza, Sapienza-Università di Roma, University of Paris VI, ETH-Zurich).

Meetings organization and other responsibilities

In April 2007 LG organized as principal and local organizer, the 3-days Workshop *"Progress in ab initio modeling of biomolecules: towards computational spectroscopy"* which was held in Rome with more than 100 participants. The workshop was founded mainly by ESF through the SimBioMa and Psi-K networks.

In September 2010 LG co-organised the Symposia "Ab-Initio Methods on Biological Systems" of the Conference "Psi-k2010" in Berlin, Germany.

In February 2011 LG organised a national PhD School on "Ab initio Molecular Dynamics" at the Physics Department of Sapienza - University of Roma.

In June 2013 LG co-organised a 5-days international PhD School on “Ab initio Molecular Dynamics for Biomolecules” in S. Stefano di Sessanio, L’Aquila, Italy.

In May 2015 LG co-organised a 3-days international workshop on “Computer simulations for condensed phase systems”, in Roma, Italy.

In 2017 LG organised the Workshops “BUUR Workshop on Natural and Artificial Photosynthesis” at the Physics Department of Sapienza - University of Roma.

In December 2018, LG co-organised a 1-day workshop on “Quantum Computing and High Performance Computing“ at CINECA computer centre in Bologna, Italy.

From 2008 to 2017 LG was Member of the Steering Committee of the European Science Foundation ESF-RNP Network Program on electronic structure “Advanced Concepts in ab-initio Simulations of Materials Psi-k2”.

In 2015 LG was member of the Research Commission of the Department of Physical and Chemical Science at the University of L’Aquila.

From 2015 LG is member of the Research Commission of the Department of Physical and Chemical Science at the University of L’Aquila.

In 2019 and 2020 LG was delegate of the Department of Physical and Chemical Science at the University of L’Aquila for the “Night of Research”.

Funding and responsibilities

Year	Title, function	Funding Agency/Program	Grant value
2020-2023	Partner Coordinator	Innovative Training Network: project Molecular Quantum Simulations	260.000 EUR
2020-2023	Project Coordinator	National Fundings for a 3-year PhD fellowship in collaboration with an industrial partner.	80.000 EUR
2019-2022	Project Coordinator	National Fundings for a 3-year PhD fellowship in collaboration with an industrial partner.	80.000 EUR
2019-2022	Project Coordinator	Regional Fundings for a 3-year Researcher. PON-AIM AIM1842894	197.000 EUR
2009-2015	Principal Investigator	European Research Council – IDEA Starting Grant. Project no. 240624 entitled “Electronic Structure of Chemical, Biochemical, and Biophysical Systems: Multiscale Approach with Electron Correlation”.	1.200.000 EUR
2010-2011	Principal Investigator	Subcontract between the Massachusset Institute of Technology (Boston, USA) and the Univ. degli studi de L’Aquila. Title: ”Quantum Monte Carlo Study of free Radicals”.	40.000 USD
2006-2007	Principal Investigator	CASPUR – two year postdoc working at caspur under LG scientific supervision	40.000 EUR (estimated)
2011-	Principal	Many Grants from the PRACE (Partnership	More than 150 million

2018	Investigator	for advanced Computing in Europe) infrastructure (peer review European call). Winner of: PRACE 3rd call, PRACE 5th call, PRACE 6th call, PRACE 7th call, PRACE 9th call, PRACE 11th call, PRACE 14th call, PRACE 16th call (continuation project).	CPU-core hours (equivalent to use 5.000 CPUS cores for 3 years). Estimated value: 200.000 EUR)
2005-present	Principal Investigator	Granted as Principal Investigator of several CPU-time national grants from the CASPUR and CINECA computer centres	

Refereeing

LG is referee for the following international journals: *Angewandte Chemie, Nature Communications, ACS Cathalysis, Biophysical Journal; Bioinformatics; Journal of Physical Chemistry; Journal of the American Chemical Society; Proteins, Structure Function and Bioinformatics; Journal of Biomolecular Structure and Dynamics; Future Generation Computer Systems, European Biophysical Journal; Journal of Chemical Theory and Computation, Biochemistry, Theoretical Chemistry Accounts, Physiologia Plantarum, Biochimica et Biophysica Acta, International Journal of Quantum Chemistry, International Journal, PLOS Computational Biology, Expert Systems with Applications.*

LG is referees for both the Physics and the Chemistry areas of the national grants (FIRB and PRIN) and the national system for the evaluation of research (VQR). He is also referee for the Europen Research Council (Junior and Senior grants), the European Science Foundation (ESF) and other National European Agencies such as L'Agence Nationale de la Recherché (ANR) in France, the Czech Science Foundation in Check Republic, the Foundation of Fundamental Research on Matter (FOM) in the Netherlands, and the U.S. Department od Energy.

Reaserch interests

Main topics

1) Development of accurate multiscale methods in Computational Chemistry.

As Principal Investigator of the ERC project MultiscaleChemBio, LG is working to overcome current limitations of computational Physics to tackle large molecular systems where the electron correlation plays a crucial role. The methodology is based on a multiscale approach based on Quantum Monte Carlo (QMC), Density Functional Theory (DFT) and Molecular Mechanics. This technique offers the advantage of a high accuracy at an affordable computational cost and can exploit the next generation massively parallel computers.

2) Applications to Molecular Simulations and Materials Science.

To aid the interpretation of experimental data we applied complementary computational techniques, such as ab-Initio Molecular Dynamics, DFT and QMC, to several systems in Biophysics (ionic channels, photosynthetic proteins, photoreceptors) Molecular Physics (molecular catalysts, metallo-organic complexes, liquids) and Materials Science (catalysis at interfaces). In the field of photoreceptors, such as Rhodopsin, GFP, PYP and PCP, our calculations were able to rationalize the role of the environment on the properties and the spectroscopy (Raman, Infrared and UV/vis) of the biological chromophores. The research activity is expanding in the field of natural and artificial photosynthesis in order to understand the light-capturing and catalytic strategies of the natural photosynthetic systems and of their synthetic analogues.

3) Quantum Chemistry algorithms for Quantum Computation.

Together with the established research lines, LG started in 2018 a research activity in the field of application of Quantum Computing to electronic structure problems. Currently one post-doc, one PhD student and one Master students are involved. The PhD has been recruited within the MIUR activity "Dottorati Innovativi con caratterizzazione industriali" in parternship with IBM-Italia. Collaborations have been established with IBM-Italia and the IBM research centre in Zurich.

Keywords: Electronic Structure calculations, Density Functional Theory, Quantum Monte Carlo, Computational Biophysics, Protein Chemistry and Protein Biophysics, Photoreceptors, Ionic Channels, Photosynthesis Research, Materials Science for Energy Research.

Current international collaborations

Scientific collaborations with the following groups are currently (mar 2016) active:

- Prof. H. Dau, Freie Universitaet, Berlin, Germany.
- Prof. Charles Des Francois, Univ. Paris XIII, France.
- Dr. Dimitrios Pantazis, MPI, Stutgard, Germany.
- Dr. Debora Scuderi, Univ. Paris Sud, France.
- Dr. Ivano Tavernelli, IBM-Research, Zurich, Switzerland.

Several collaborations are currently active with different Experimental and Theoretical groups from Italian universities in different fields (Physics, Chemistry, Pharmacology, Bioinformatics)

Awards

Jul 2002	Lugano, Switzerland	Best Poster Presentation Award *at the 6th World Congress of Theoretically Oriented Chemists.*
Jun 2000	Genova, Italy	Young author award *of the National Conference on Physics of Matter.*

Talks and seminars

Feb 2022	Online	**Invited seminar** at the Thematic afternoon on quantum algorithms for chemistry at Department of Chemistry of University of Strasbourg: *"Quantum Chemistry algorithms on near-term devices".*
Oct2021	Online	**Invited talk** at the Computational Photosynthesis 2021 meeting: *"Hills and valleys on the Kok-Joliot cycle"*
Oct 2020	Online	**Invited talk** at the BUUR Special on water oxidation in PSII: *"Pathway for water oxidation in PSII".*
Feb 2020	Padova, Italy	**Invited seminar** at the Department of Chemistry of Padua University**:** *"Quantum Chemistry with Quantum Computers".*
Dec 2020	Bologna, Italy	Selected speaker at the second Workshop on High-Performance Computing and Quantum Computing: "*Extended Variational Quantum Eigensolver".*
Jul 2019	Marseille, France	**Keynote speaker** at the *Quantum Bioinorganic Chemistry Conference*: "Structure, reactivity and dynamics of biological and synthetic Multi-Centers Transition Metal clusters"
Jul 2019	Rome, Italy	**Keynote speaker** at the XLVII Congress of the Chemical Physics Division: *Quantum Chemistry using Quantum Computers.*
Jun 2019	Paris, France	**Invited speaker** at the workshop of the French Society of Photosynthesis: "*Modelling the water splitting reaction in Photosystem II*".
Feb 2019	Rome, Italy	**Invited talk** at the workshop on *Bioinformtics applications in Life Science*, Università di Roma3.
Nov 2018	Rome, Italy	**Invited talk** at the Annual Meeting on Computational and System Biology of the *Italian Society of Biochemistry and Molecular Biology*: "Atomistic simulations in Biology".
Oct 2018	Rome, Italy	**Invited talk** at the Workshop *Computer Simulation in the Physical and Life Science* at Temple University Rome: "Modelling molecular mechanisms in photosynthesis".
Oct 2018	Berlin, Germany	**Invited seminar** at the Freie Universitaet: "Molecular Simulations in Photosynthesis".
Jun 2018	Uppsala, Sweden	**Invited talk** at the First European Conference on Photosynthesis: "Structural and electronic insights on the catalytic mechanisms of Photosystem II".
Feb 2018	Helsinki, Finland	Talk at the *University of Helsinki*: "Modelling the molecular mechanisms of Photosynthesis".
Jul 2017	La Jolla, USA, CA	Short Talk at the *2nd International Solar Fuels Conference (ISF-2*): "Modelling Intermediate States Along the Catalytic Cycle of Photosystem II".
Jul 2017	La Jolla, USA, CA	Seminar at the Scripps research institute, Dept. of Chemistry: "Modelling Transition Metal Clusters in Enzymes: Applications and Computational Perspectives".
May 2017	Rome, Italy	Contributed talk at the meeting *Biophysics@Rome 2017:* "The molecular details of the first steps in photosynthesis"
Apr 2017	Rome, Italy	**Invited outreach speech** at *Floracult 2017:* "Fotosintesi Naturale e Foglie Artificiali"
Apr 2017	Rome, Italy	Contributed talk at the *BUR meeting on natural and artificial photosynthesis*: "Molecular Vibrations of a Synthetic Mn4Ca cluster"
Sep 2016	Cortona, Italy	**Invited talk** at the *XXIII National Congress of the Italian Society of Pure and Applied Biophysics (SIBPA):* "The molecular mechanisms of photosynthesis by ab initio molecular dynamics"
Sep 2016	Lausanne, Switzerland	**Invited talk** at the *CECAM Workshop Interface processes in photochemical water splitting: Theory meets experiment.*
May 2016	Pisa, Italy	**Invited talk** at the *CECAM Workshop Structural and Functional Annotation of Bioinorganic Systems: Perspectives and Challenges from Theory and Experiments.*
Apr 2016	London,	Seminar at the *University College London*: "Modeling the

	United Kingdom	molecular mechanisms of water splitting in oxygenic photosynthesis".
Apr 2016	Oxford, United Kingdom	**Invited talk** at the *Isolated Biomolecules and Biomolecular Interactions Conference 2016*: "Modelling the Molecular Mechanisms of Photosynthetic Water Splitting".
Feb 2016	Florence, Italy	Contributed talk at the *1st Enerchem Congress*.
Dec 2015	Roma, Italy	Contributed talk at the workshop of the *Computational Chemistry division of the Italian Chemical Society*: "Accurate Quantum Chemistry for Exascale Computing".
Nov 2015	Engelberg, Switzerland	**Invited talk** at the *COST action PERSPECT H2O*: "Ab initio molecular dynamics in photosynthetic water splitting".
Nov 2015	Uppsala, Sweden	Contributed talk to the *BUUR Meeting 2015*:" Vibrational fingerprints of the Mn4CaO5 cluster in Photosytem II by first principles molecular dynamics".
Oct 2015	Roma, Italy	Contributed talk at the conference *PHOTOTECH 2015: Towards a photosynthesis-biobased economy:" Structure and Reactivity of Water Splitting Catalysts in Natural and Artificial Photosynthesis".*
Sep 2015	Palermo, Italy	**Invited talk** at the conference *FisMat 2015*: "Exploring the molecular mechanisms of photosynthesis by ab initio molecular dynamics"
Sep 2015	San Sebastian, Spain	**Invited talk** at the *Psi-k 2015 conference 2015*: "Quantum Monte Carlo on biomolecules".
Jul 2015	Torino, Italy	**Invited keynote talk** at the *Congress of Theoretical Chemists of Latin Expression (CHITEL2015):*" Molecular Structures and Ab Initio Molecular Dynamics by Many Particle Quantum Mechanics "
Jul 2015	Roma, Italy	Contributed talk at the *Italian Meeting on Porphyrins and Ptalocyanines – 2:* "The Special Pair of Chlorophylls in Photosynthesis. Insights by Computer Simulations".
Jun 2015	Telluride, CO, USA	**Invited talk** at the *Stochastic Electronic Structure* workshop: "Molecular Properties of (Bio)molecules by Quantum Monte Carlo".
May 2015	Roma, Italy	Contributed talk to the conference *Biophysics@Rome 2015*: "Exploring the molecular mechanisms of photosynthesis by ab initio molecular dynamics".
Apr 2015	Uppsala, Sweden	Contributed talk at the *1st International Solar Fuels Conference (ISF-1):*" Structure and reactivity of water splitting catalysts by computer simulations".
Mar 2015	Umea, Sweden	**Invited talk** at the *Umea Workshop on Renewable Energy*: "Simulating photosynthetic processes in Photosystem II by first principles".
Jan 2015	Venice, Italy	**Invited lecture** at the *XIX School of Pure and Applied Biophysics*: "Quantum Mechanics / Molecular Mechanics simulations in Biophysics".
Oct 2014	Amsterdam, The Netherlands	**Invited talk** at the *Workshop on Photosynthesis*, Free University of Amsterdam: "Ab initio molecular dynamics of Photosystem II".
Aug 2014	Berkeley, CA, USA	Seminar at the Chemistry Department: "Molecular geometries and dynamics of large systems by Quantum Monte Carlo"
Aug 2014	Pasadena, CA, USA	**Invited seminar** at the *Chemistry Department of the California Institute of Technology (CALTECH):* "Molecular mechanisms of Natural and Artificial water splitting"
Aug 2014	Mount Snow, VT, USA	**Invited talk** at the *Gordon Conference on Photosynthesis*: "Molecular Pathways From S2 to S3 States of Photosystem II Explored by Ab Initio QM/MM Dynamics"
Aug 2014	New York, USA	**Invited seminar** at *New York University*: "Molecular Structures and Dynamics by Quantum Monte Carlo".
Aug 2014	Philadelphia, USA	**Invited seminar** at the Temple University: "Ab initio molecular dynamics in natural and artificial photosynthesis".
Aug 2014	Princeton, USA	**Invited seminar** at the Princeton University: "Quantum

		Monte Carlo for Correlated (Bio)molecules and Ab Initio Molecular Dynamics".
Jul 2014	Apuan Alps, Italy	Contributed talk at the *QMC workshop on the Apuan Alps IX*: "Geometries and properties of (bio)molecules by Quantum Monte Carlo".
Jun 2014	Oslo, Norway	**Invited talk** at the *FemEx-Oslo conference*: "Electrons and protons on the way to photosynthetic water splitting"
Jun 2014	London, United Kingdom	Contributed talk at the workshop at *University College London* on *Interface between experimental and theoretical approaches to energy-related enzyme catalysis:* "Movements of protons and electrons along the pathway for water splitting in the Oxygen Evolving Complex of Photosystem II"
Jun 2014	London, United Kingdom	**Invited seminar** at the *King's College London*: "Geometrical and electronic properties of correlated (bio)molecules by Quantum Monte Carlo"
May 2014	Rome, Italy	Contributed talk at the conference: *Biophysics@Rome*: "The molecular biophysics of photosynthesis explored by first principles"
Sep 2013	Pisa, Italy	Contributed talk at the *Avogadro Colloquia*: "Ab Initio Molecular Dynamics in Artificial and Natural Photosynthesis"
Sep 2013	Lille, France	Invited talk at the Conference *EMLG-JMLG - Global perspectives on the structure and Dynamics of liquid and mixtures: experiment and simulation*: "Spectroscopic and structural properties of liquids and solutions from ab initio molecular dynamics"
Sep 2013	London, United Kingdom	**Invited seminar** at the *King's College London*: "Ab Initio Molecular Dynamics in Artificial and Natural Photosynthesis"
Apr 2013	Berlin, Germany	Invited talk at the *First Colloquium of the Collaborative Research Center on Protonation Dynamics in Protein Function, (Freie Univ.)*: "Ab Initio Molecular Dynamics in Artificial and Natural Photosynthesis"
Mar 2013	Pisa, Italy	**Invited seminar** at the *Chemistry department of the University of Pisa*: "Quantum Monte Carlo as emerging tool to access electronic and geometrical properties of correlated biomolecules"
Oct 2012	Kobe, Japan	**Invited talk** to the Conference on Computational Physics 2012: "Tackling the electron correlation in biomolecules by Quantum Monte Carlo / Molecular Mechanics"
Sep 2012	Chia, Italy	Contributed talk to the Conference *Energy from the Sun: Computational Chemists and Physicists Take up the Challenge*:
Jun 2012	Firenze, Italy	Contributed talk at the *XVIII National Congress of Industrial Chemistry:* "Modelling the electronic structure of artificial photosynthesis: structure and reactivity of a cobalt-based catalyst for water oxidation"
Oct 2011	Berlin, Germany	**Invited seminar** at the *Physics Department of the Freie Universitaet*: "Geometry relaxation and vibrational spectroscopy by Quantum Monte Carlo"
Sep 2011	Lecce, Italy	**Invited talk** at the *Italian Chemical Society Conference*: "Perspectives in Electronic Structure of Chemical and Biochemical Systems: Multiscale Approach with Electron Correlation"
Sep 2011	Barcelona, Spain	**Invited talk** to the Conference: *"Car-Parrinello Molecular Dynamics 2011"*: "Vibrational spectroscopy by Quantum Monte Carlo"
Jun 2010	Lugano, Switzerland	Contributed talk to the *CECAM workshop "Quantum Monte Carlo meets Quantum Chemistry: new approaches for electron correlation"*: "Stucture and harmonic frequencies of the water molecule by Quantum Monte Carlo".
Mar 2010	Berlin, Germany	Contributed talk to the *Solar-H2 workshop*: "Quantum Mechanics / Molecular Mechanics simulations of biological systems"

Sep 2009	Alba Adriatica, Italy	**Invited talk** at the intensive program Mathematical Models in Life and Social Sciences
Sep 2009	Palermo, Italy	Contributed talk a the European Conference on the Spectroscopy of Biological Molecules "Structure and reactivity of a cobalt-based catalyst for water oxidation"
Sep 2009	San Sebastian, Spain	**Invited talk** at the Summer School on Simulation Approaches to Problems in Molecular and Cellular Biology
May 2007	Roma, Italy	**Invited seminar** at the *University of Roma La Sapienza, Dept. of Chemistry*: "Electronic properties of biomolecules by first principles"
Apr 2007	Roma, Italy	**Invited seminar** at the *University of Roma La Sapienza, Dept. of Mathematics*: "Exploring biological systems by classical and quantum molecular simulations"
Dec 2006	Roma, Italy	**Invited seminar** at the *University of Roma Tor Vergata*: "Exploring Biological Systems by First Principles: QM/MM and Quantum Monte Carlo"
Dec 2006	Trento, Italy	**Invited talk** at the *workshop on Quantum Monte Carlo Methods*: "Simulating biological systems by Quantum Monte Carlo"
Jul 2006	Leiden, The Netherlands	Contributed talk to the *Psi-k workshop 'Progress in ab initio modeling of biomolecules: methods and applications'*: "Absorption Spectra by QMC/MM"
May 2006	Bertinoro, Italy	**Invited talk** to the workshop *Perspectives on Science and Engineering Driven Supercomputing*: "High Performance Computing in Biophysics and Biochemistry"
May 2006	Lyon, France	Cotributed talk to the CECAM Workshop *'New developments for first principles MD simulations in condensed matter and Molecular physics'*: "Absorption Spectra in Solution by QMC/MM Simulations"
May 2006	Gaeta, Italy	**Invited talk** to the *5th Workshop on Molecular Theories and Simulations*: "Calculating absorption spectra of biomolecules: QM/MM, TDDFT and Quantum Monte Carlo"
Feb 2006	Roma, Italy	Contributed talk to the conference *ABR06*: "First Principles Quantum Mechanics/Molecular Mechanics (QM/MM) Simulations of Biological Systems"
Oct 2005	Rimini, Italy	**Invited talk** to the *3rd National Congress on Chemistry of Biological Systems*: "Quantum Monte Carlo as high accuracy computational method for Biological Chemistry"
Sep 2005	Scwäbisch Gmünd, Germany	Contributed talk to the *Psi-k 2005 Conference*: "Absorption spectra in solution: combining Quantum Monte Carlo with Car-Parrinello Dynamics"
Jul 2005	Roma, Italy	Contributed talk to the *European Symposium on Organic Reactivity*: "Electronic reaction coordinates"
May 2005	Gaeta, Italy	**Invited talk** to the *4th Workshop on Molecular Theories and Simulations*: "Ab initio Quantum Mechanics / Molecular Mechanics Simulations of biological systems"
Sep 2004	Genova, Italy	Contributed talk to the *Conference on Computational Physics*: "Accelerating Chemical Reactions in mixed Quantum/Classical Simulations by Biasing Molecular Orbitals"
Feb 2003	Trieste, Italy	**Invited Seminar** at the *Democritos INFM Center*: "Molecular Mechanisms of light Detection in Rhodopsin".
Nov 2003	Modena, Italy	**Invited Seminar** at the *S3 INFM Center*: "Classical and Mixed QM/MM dynamics in biological and biomimetic systems".
Oct 2003	Lausanne, Switzerland	Contributed talk to the *Swiss Chemical Society Fall Meeting 2003*: "Driving Chemical Reactions via Biases of Molecular Orbitals".
Feb 2003	Frascati, Italy	Contributed talk to conference *Advances in Experimental and Theoretical Methods for Biological Application of Synchrotron Radiation (BioSR)*: "QM/MM Simulations of Rhodopsin: Insights into the Early Steps of Light Detection in the Eye.

Nov 2002	Bern, Switzerland	Biochemistry Seminar at the *University of Bern*, invited by Prof. B. Erni: "Exploring biological systems by quantum and molecular mechanics simulations".
Nov 2002	Basel, Switzerland	Physical Chemistry Seminar at the *University of Basel*, **invited** by Prof. H. Huber: "Ab initio and molecular mechanics simulations of biological systems".
Apr 2002	Roma, Italy	Contributed talk to the conference *Acta Biophysica Romana 2002*: "Simulating the molecular mechanisms of membrane proteins: ionic channels and photoreceptors".
Sep 2001	Manno, Switzerland	Contributed talk at the *CSCS users day*: "Mixed Quantum/Classical QM/MM Car-Parrinello simulations in biological sistems".
Jun 2001	Roma, Italy	Contributed talk to the *National Conference of Physics of Matter*: "Modeling permeation and blocking in potassium channels".
Mar 2001	Roma, Italy	Seminar at the physics department of *Universitá di Roma "La Sapienza",* invited by Prof. A. Congiu-Castellano: "Ionic channels: permeation and blocking mechanisms".
Feb 2001	Boston, MA (USA)	Contributed talk to the *Biophysical Society 45th Annual Meeting* (*Biophys. J.* 80, A175 (2001)): "Barrier crossing in the selectivity filter of KcsA potassium channel".
Oct 2000	Parma, Italy	**Invited talk** at the *XV Meeting of the Italian Society of Pure and Applied Biophysics (SIBPA 2000)*: "Theoretical studies on the KcsA potassium channel ".
Mar 2000	Rome, Italy	Seminar at the physics department of *Universitá di Roma "La Sapienza",* invited by Dr. A. Giansanti: "Ionic channels: from the first crystal to molecular dynamics".
Feb 2000	New Orleans, LA (USA)	Contributed talk to the *Biophysical Society 44th Annual Meeting* (*Biophys. J.* 78, A138 (2000)): "Hydration and dynamics of the K^+ channel".
May 1999	Trieste, Italy	Contributed talk at the *Workshop on Phototransduction and Chemotransduction organized by the consortium of E.C. Biotech Project*: "The KcsA potassium channel: microscopic and dynamical properties".
Feb 1999	Charlottesville, VA (USA	Seminar at the *University of Virginia Health Sciences Center*, **invited** by E. Perozo: "K^+ channel tetrameric stability explored by molecular dynamics simulations".
Feb 1999	Baltimore, MD (USA)	Contributed talk to the *Biophysical Society 43rd Annual Meeting* (*Biophys. J.* 76, A153 (1999)): "K^+-potassium channel interactions explored by molecular dynamics simulation".
Nov 1998	Miami, FL (USA)	Contributed talk to the *43rd Annual Conference on Magnetism and Magnetic Materials*: "Spin gap in low-dimensional Mott insulators with orbital degeneracy".

Leonardo Guidoni - Publications

According the Scopus database the **100** publications of Leonardo Guidoni received totally more then **3000** citations and an H-index of **32**.

Impact factors (**IF**) are reported from Journal Citation Reports. For references 1-10 (2017-2019) have been considered the Impact Factors of year 2016. For references 76 and 83 the Impact Factors were not available for the specific years and have been reported those of the next years. For all the other references are reported the year-specific Impact Factors of each journal. Citations count is reported from Scopus.

Journals

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2. Nakamura S., Capone M., Narzi D. and Guidoni L., *Pivotal role of the redox-active tyrosine in driving the water splitting catalyzed by Photosystem II*, **(2020) *Physical Chemistry Chemical Physics*** *22, 273,* DOI: 10.1039/C9CP04605D

3. Frezzini M., Guidoni L. and Pascarella S., *Conformational transitions induced by γ-amino butyrate binding in GabR, a bacterial transcriptional regulator,* **(2019) Scientific Reports** 9, 19319, DOI: 10.1038/s41598-019-55581-1.

4. Tichengulova A., Capone M., Pitari F., Guidoni L., *Molecular vibrations of Oxygen-Evolving Complex and its synthetic mimic*, **(2019) Chemistry, a European Journal**, DOI: 10.1002/chem.201902621. **IF: 5.160**.
5. Capone M., Narzi D., Tychengulova A., Guidoni L. *On the comparison between differential vibrational spectroscopy spectra and theoretical data in the carboxyl region of photosystem II.* **(2019) Physiologia plantarum** 166, 33-43, DOI: doi.org/10.1111/ppl.12949. **IF: 2.580**.

6. Pasquini C., Zaharieva I., Gonzalez-Flores D., Chernev P., Mohammadi M., Guidoni L, Smith R. and Dau Holger, *H/D Isotope Effects Reveal Factors Controlling Catalytic Activity in Co-Based Oxides for Water Oxidation*, **(2019) Journal of the American Chemical Society**, 141, 7, 2938-2948, DOI: 10.1021/jacs.8b10002. **IF: 14.357**.

7. Capone M., Narzi, D., Tychengulova, A., Guidoni, L., *On the comparison between differential vibrational spectroscopy spectra and theoretical data in the carboxyl region of Photosystem II*, **(2019) Physiologia Plantarum**, DOI: 10.1111/ppl.12949. **IF: 3.656**.

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9. Corinti, D., Gregori, B., Guidoni, L., Scuderi, D., McMahon, T.B., Chiavarino, B., Fornarini, S., Crestoni, M.E. *Complexation of halide ions to tyrosine: Role of non-covalent interactions evidenced by IRMPD spectroscopy*. **(2018) Physical Chemistry Chemical Physics**, 20 (6), pp. 4429-4441. DOI: 10.1039/c7cp06657k. **IF: 4.123.**

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