Curriculum Vitae

Emanuele Coccia

Personal Details

Name: Emanuele Coccia
Date of birth: 7/1/1982
Place of birth: Rome (Italy)
Citizenship: Italian
Languages: Italian, English, French
Email: ecoccia@units.it, emanuele.coccia82@gmail.com

Academic positions

Dec, 21 2018 - Assistant Professor (*Ricercatore a tempo determinato di tipo B CHIM/02 03/A2*) at the Department of Chemical and Pharmaceutical Sciences, University of Trieste.

Aug, 3 2018 - Dec, 16 2018 Fixed-term researcher (*Ricercatore a tempo determinato di tipo A CHIM/02 03/A2*) at the Department of Chemical Sciences, University of Padova, within the EU grant ERC-CoG-2015 No. 681285 "TAME-Plasmons: a Theoretical Chemistry Approach to Time-Resolved Molecular Plasmonics" by Prof. Corni.

Dec, 1 2016 - Aug, 2 2018 Post doctoral position at the Institute of Nanoscience, S3 CNR Nano, Modena (until 31, Oct 2017) and at the Department of Chemical Sciences, University of Padova, under the supervision of Prof. Corni. Project: *Development of hybrid quantum-chemical and time-dependent models for molecules close to metal nanoparticles*, funded by EU grant ERC-CoG-2015 No. 681285 "TAME-Plasmons: a Theoretical Chemistry Approach to Time-Resolved Molecular Plasmonics".

Nov, 15 2014 - Nov, 30 2016 Post doctoral position at the Laboratoire de Chimie Theorique, Université Pierre et Marie Curie & CNRS, Paris (and partial support from the Department of Physical and Chemical Sciences, University of L'Aquila) under the supervision of Dr. Luppi and Toulouse. Project: *High-harmonic generation in atoms and small molecules interacting with intense fields*, funded by Labex MICHEM part of French state funds managed by the ANR within the Investissements d'Avenir programme under reference ANR-11-IDEX-0004-02.

Nov, 1 2011- Oct, 31 2014 Post doctoral position at the Department of Physical and Chemical Sciences, University of L'Aquila under the supervision of Prof. Guidoni. Project: *Multiscale simulations using quantum Monte Carlo methods*, funded by the grant ERC "MultiscaleChemBio" (n. 240624) within the VII Framework Program of the European Union.

Apr, 1 2010 - Oct, 31 2011 Post doctoral position at the Department of Chemistry, Chemical Engineering and Materials, University of L'Aquila under the supervision of Prof. Guidoni. Project:

Electronic-structure calculations for strongly correlated systems using quantum Monte Carlo methods, funded by the grant ERC "MultiscaleChemBio" (n. 240624) within the VII Framework Program of the European Union.

Education and scientific profile

Dec 2018	Participation to the workshop "Quantum Computing and High Performance Computing" at CINECA, Casalecchio di Reno (Italy)
Apr 2018	*Abilitazione Scientifica Nazionale per Professore di seconda fascia nel settore 03/B1 (Fondamenti delle Scienze Chimiche e Sistemi Inorganici)* (Italian qualification for associate professor in General and Inorganic Chemistry)
Feb 2018	Participation to the *Winter College on Extreme Non-linear Optics, Attosecond Science and High-field Physics* at the ICTP, Trieste (Italy)
Dec 2017	*Abilitazione Scientifica Nazionale per Professore di seconda fascia nel settore 03/A2 (Modelli e Metodologie per le Scienze Chimiche)* (Italian qualification for associate professor in Physical Chemistry)
Feb 2016	*Qualification aux fonctions de maitre des conférences* (French qualification for academic positions) for Theoretical, Physical and Analytical Chemistry
May 2014	Participation to the *Hands-on Tutorial on Excited State Spectroscopy: GW and BSE using the Yambo code* at CINECA, Rome (Italy)
Feb 2011	Participation to the *Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) Approaches to Biochemistry (and beyond)* at CECAM, Lausanne (Switzerland)
Oct 2010	Participation to the *Hands-on workshop on excitations in solids and nano-structures from first-principles* at the SISSA, Trieste (Italy)
Dec 2009	Final PhD exam. Thesis title: *Chemical solutions in a quantum solvent: a study of doped helium clusters* (final judgment: *altamente meritevole*, highly deserving)
Jan 2008	Participation to the *Advanced School on Quantum Monte Carlo Methods in Physics and Chemistry* at the ICTP, Trieste (Italy)
Dec 2007	Participation to the *Introduction to HPC: parallel computing*, CASPUR, Rome (Italy)
Nov 2007	Participation to the *Introduction to HPC: high performance computing*, CASPUR, Rome (Italy)
Nov, 1 2006	PhD position in the theoretical chemistry group at the University of Rome "Sapienza" (supervisor: F. A. Gianturco)
Oct, 27 2006	Master degree in Chemistry Magna cum Laude (final judgment: 110/110 *e lode*, maximum in Italian University) at the University of Rome "Sapienza". Dissertation title: *Stochastic methods for the determination of ionic microsolvation in quantum solvents*
Nov, 11 2004	Bachelor degree in Chemistry Magna cum Laude (final judgment: 110/110 *e lode*, maximum in Italian University) at the University of Rome "Sapienza". Dissertation title: *Algoritmi stocastici per sistemi di Van der Waals: il codice DMC per lo studio di molecole di p-H_2 in gocce di elio*

Research activity

Stochastic approaches for open systems: real-time approaches for plasmonic systems. The theory of open systems is successful in describing the effect of the environment on a given quantum system, as, for instance, dephasing (i.e. loss of coherence). Revealing possible long-living quantum coherence in ultrafast processes allows detecting genuine quantum mechanical effects in molecules. To investigate such effects from a quantum chemistry perspective, we have developed a method for the time evolution of molecular systems based on ab initio calculations that include the effect of an environment, in terms of dephasing of the molecular wave function, and relaxation. Such effects are accounted for by means of the stochastic Schrödinger equation (SSE) technique. We exploit a computational protocol based on the real-time propagation of the time-dependent electronic wave function, expanded in configuration-interaction eigenstates of the molecular target. SSE is implemented in a multiscale model describing the interaction between a molecule (treated at quantum level of theory) and a dielectric medium (solvent or metal nanoparticle). Three different interaction channels with the environment are proposed: relaxation to the ground state by means of spontaneous emission, nonradiative relaxation through internal conversion and pure dephasing of the wave function. The propagation of the SSE is performed by using a quantum jump algorithm.
To test the approach, we have simulated femtosecond pulse-shaping ultrafast spectroscopy of terrylenediimide (TDI). TDI emission is strongly affected by the dephasing induced by the environment. This effect is investigated by changing the delay time and the relative phase shift between the two pulses. Our results reproduce the experimental findings [R. Hildner *et al.*,Nature Phys., **7**, 172 (2011)] (**Article 31**).
We also studied a model chromophore (LiCN) interacting with a spherical silver nanoparticle, both embedded in an external environment determining dephasing of the molecular wave function. Attention has been focused on how absorption properties of LiCN change with the distance between the molecule and the nanoparticle, and how dephasing affects the plasmonic features of the "super-absorber" composed of LiCN+nanoparticle.
*High-harmonic generation.*This research activity involves the real-time theoretical study of non-linear effects in the interaction between atomic and molecular systems and strong laser fields. In particular, I apply time-dependent configuration interaction to solve the time-dependent Schrödinger equation for the study of high-harmonic generation, specifically focusing the attention on the construction of reliable Gaussian basis sets for the continuum and on the definition of accurate procedures for taking into account electron loss during the time propagation (**Articles 22, 23, 27 and 33**).
QMC for biochromophores. My research activity is also focused on the use of Quantum Monte Carlo (QMC) methods for the study of the electronic and structural properties of molecules of biological interest, like chromophores involved in the mechanism of vision (retinal protonated Schiff base), in energy transfer in the initial step of the photosynthetic process (peridinin carotenoid) or in bioluminescence (anionic forms of oxyluciferin). I am specifically interested in the development of hybrid QMC/MM schemes in order to investigate the net effect of an external (protein) environment on the target molecule, giving a special attention to the tuning of some key geometrical properties of the chromophore (like the bond length alternation of the polyenic chain characterizing such systems) due to the interaction with the protein. Excited states of such molecular systems are investigated by means of TDDFT, wave function and Many Body Green's Function Theory approaches. (**Articles 15-17, 19, 20, 25 and 30**)
JAGP ansatz for diradicals. I am also interested in the investigation of the intrinsic properties of the Jastrow Antisymmetrised Geminal Power ansatz (JAGP) for the study of diradical systems (as the orthogonally twisted ethylene molecule, the methylene and the tetramethyleneethane), of the thermal isomerization of the minimal model of the retinal, where static (strong) correlation plays an essential role, and of linear response properties, as the static polarizability. (**Articles 14, 18, 20 and 21**)
Photosynthesis. QMC methods have been also applied to the study of the thermodynamics of the water splitting reaction, based on a cobalt model as catalyst (**Article 24**). Site-energy shifts of chlorophylls in

Photosystem II along a classical molecular dynamics have been computed (**Article 29**).
QMC for excited states. QMC has been extended to the calculation of electronic excited states by means of linear response theory (**Article 28**).
QMC for helium clusters. I worked on the development and applications of QMC methodologies for the study of doped ^{4}He clusters. Different types of impurities were studied: cationic (alkali metal ions and dimers) inducing a strong localization of the helium atoms, neutral (H, H_2, Li_2 and Cs_2) showing only a weak coupling with the "solvent" and anionic systems (OH^-, halogen anions) that are embedded but do not produce a clear structure in the cluster. (**Articles 1-13**) The extension of DMC to the calculation of rotational excited states of doped He clusters is applied to the $CO(^4He)_N$ system (**Article 26**).

Publications

Coauthor of 35 publications on international journals, with 447 citations and h-index equal to 15 on Scopus (Sep 23rd 2019). 510 citations and h-index equal to 15 on Google Scholar (Sep 23rd 2019). Author ID on Scopus: 24480759400. Asterisk indicates corresponding authorship (10). Among the 35 publications, 1 review (article 25), 1 ACS Editors' Choice (article 20) and 1 volume cover (article 8).

35. (*) E. Coccia and E. Luppi: Theor. Chem. Acc., **138** (2019), 96, *Detecting the minimum in argon high-harmonic generation spectrum using Gaussian basis sets*

34. E. Coccia and S. Corni: J. Chem. Phys., **151** (2019), 044703, *Role of coherence in the plasmonic control of molecular absorption*

33. M. Labeye, F. Zapata, E. Coccia, V. Véniard, J. Toulouse, J. Caillat, R. Taieb, E. Luppi: J. Chem. Theory. Comput., **14** (2018), 5846, *On the optimal basis set for electron dynamics in strong laser fields: The case of molecular ion* H_2^+

32. J. Fregoni, G. Granucci, E. Coccia, M. Persico, S. Corni: Nat. Commun., **9** (2018), 4688, *Manipulating azobenzene photoisomerization through strong light-molecule coupling*

31. (*) E. Coccia, F. Troiani, S. Corni: J. Chem. Phys., **148** (2018), 204112, *Probing quantum coherence in ultrafast molecular processes: an ab initio approach to open quantum systems*

30. (*) B. Mussard, E. Coccia, R. Assaraf, M. Otten, C. J. Umrigar, J. Toulouse: Adv. Quantum Chem., **76** (2018), 255, *Time-dependent Linear-Response Variational Monte Carlo*

29. (*) E. Coccia, D. Varsano, L. Guidoni: J. Chem. Theory Comput., **13** (2017), 4357, *Theoretical* $S_1 \leftarrow S_0$ *absorption energies of the anionic forms of oxyluciferin by Variational Monte Carlo and Many Body Green's Function Theory*

28. D. Narzi, E. Coccia, M. Manzoli, L. Guidoni: Biophys. Chem., **229** (2017), 93 *Impact of molecular flexibility on the site energy shift of chlorophylls in Photosystem II*

27. E. Coccia, R. Assaraf, E. Luppi, J. Toulouse: J. Chem. Phys., **147** (2017), 014106, *Ab initio lifetime correction to scattering states for time-dependent electronic-structure calculations with incomplete basis sets*

26. (*) E. Coccia: J. Low. Temp. Phys., **188** (2017), 22, *Excited rotational states in doped* ^{4}*He clusters: a diffusion Monte Carlo analysis*

25. (*) D. Varsano, S. Caprasecca, E. Coccia: J. Phys.: Condens. Matter, **29** (2017), 013002, *Theoretical description of protein field effects on electronic excitations of biological chromophores* (**Review**)

24. S. Chu, E. Coccia, M. Barborini, L. Guidoni: J. Chem. Theory Comput., **12** (2016), 5803, *Role of Electron Correlation along the Water Splitting Reaction*

23. (*) E. Coccia, B. Mussard, M. Lebeye, J. Caillat, R. Taieb, J. Toulouse, E. Luppi: Int. J. Quant. Chem., **116** (2016), 1120, *Gaussian continuum basis functions for calculating high-harmonic generation spectra*

22. (*) E. Coccia and E. Luppi: Theor. Chem. Acc., **135** (2016), 43, *Optimal-continuum and multicentered Gaussian basis sets for high-harmonic generation spectroscopy*

21. (*) M. Barborini and E. Coccia: J. Chem. Theory Comput., **11** (2015), 5696, *Investigating disjoint non-Kekulé diradicals with quantum Monte Carlo: the tetramethyleneethane molecule through the Jastrow Antisymmetrized Geminal Power wave function*

20. (*) A. Zen, E. Coccia, S. Gozem, M. Olivucci, L. Guidoni: J. Chem. Theory Comput., **11** (2015), 992, *Quantum Monte Carlo Treatment of the Charge Transfer and Diradical Electronic Character in a Retinal Chromophore Minimal Model* (**ACS Editors' Choice**)

19. D. Varsano, E. Coccia, A. Mosca Conte, O. Pulci, L. Guidoni: Comp. Theor. Chem., **1040-1041** (2014), 338 *Ground state structures and electronic excitations of biological chromophores at Quantum Monte Carlo / Many Body Green's Function Theory level*

18. A. Zen, E. Coccia, Y. Luo, S. Sorella, L. Guidoni: J. Chem. Theory Comput., **10** (2014), 1048, *Static and dynamical correlation in diradical molecules by Quantum Monte Carlo using the Jastrow Antisymmetrized Geminal Power ansatz*

17. E. Coccia, D. Varsano, L. Guidoni: J. Chem. Theory Comput., **10** (2014), 501, *Ab initio geometry and bright excitation of carotenoids: Quantum Monte Carlo and Many Body Green's Function Theory calculations on peridinin*

16. E. Coccia, D. Varsano, L. Guidoni: J. Chem. Theory Comput., **9** (2013), 8, *Protein field effect on the dark state of 11-cis Retinal in Rhodopsin by Quantum Monte Carlo / Molecular Mechanics*

15. E. Coccia, L. Guidoni: J. Comput. Chem., **33** (2012), 2332, *Quantum Monte Carlo study of the Retinal Minimal Model* $C_5H_6NH_2^+$

14. E. Coccia, O. Chernomor, M. Barborini, S. Sorella, L. Guidoni: J. Chem. Theory Comput., **8** (2012), 1952, *Molecular Electrical Properties from Quantum Monte Carlo Calculations: Application to Ethyne*

13. E. Coccia, F. A. Gianturco: J. Phys. Chem A **114** (2010), 3221, *Attachment energetics of quantum dopants in a weakly interacting quantum solvent:* ^1H, ^2H *and* ^3H *in small* ^4He *clusters*

12. S. Orlandini, E. Coccia, I. Baccarelli, F. A. Gianturco, E. Garrido, T. Gonzalez-Lezana, G. Delgado-Barrio, P. Villarreal: Mol. Phys. **108** (2010), 57, *Binding He atoms to hydrogen moieties: quantum features from ultraweak interactions*

11. R. Prosmiti, G. Delgado-Barrio, P. Villarreal, E. Yurtsever, E. Coccia, F. A. Gianturco: J. Phys. Chem A **113** (2009), 14718, *Structuring a quantum solvent around a weakly bound dopant: the He-*Cs_2 *(*$^3\Sigma_u$*) complex*

10. S. Bovino, E. Coccia, E. Bodo, D. Lopez Duran, F. A. Gianturco: J. Chem. Phys. **130** (2009), 224903, *Spin-driven structural effects in alkali doped* ^4He *clusters from quantum calculations*

9. E. Coccia, E. Bodo, F. A. Gianturco: J. Chem. Phys. **130** (2009), 094906, *Size-dependent solvation of p-*H_2 *in* ^4He *clusters: A quantum Monte Carlo analysis*

8. E. Coccia, F. Marinetti, E. Bodo, F. A. Gianturco: ChemPhysChem **9** (2008), 1323, *Chemical Solutions in a Quantum Solvent: Anionic Electrolytes in ^{4}He Nanodroplets* **(Cover Picture)**

7. E. Coccia, F. Marinetti, E. Bodo, F. A. Gianturco: J. Chem. Phys. **128** (2008), 134511, *Anionic microsolvation in helium droplets: $OH^-(He)_N$ structures from classical and quantum calculations*

6. E. Coccia, E. Bodo, F. Marinetti, F. A. Gianturco, E. Yurtsever, M. Yurtsever, in *Latest Advances in Atomic Cluster Collisions*, Imperial College Press (2008)

5. E. Coccia, E. Bodo, F. A. Gianturco: EuroPhys. Lett. **82** (2008), 23001, *Nanoscopic phase changes in doped ^{4}He droplets*

4. E. Bodo, E. Coccia, D. Lopez Duran, F. A. Gianturco: Phys. Scripta **76** (2007), C104, *Ionic dopants in He droplets: cluster energies from a variational and Diffusion Monte Carlo approach*

3. F. Marinetti, Ll. Uranga Piña, E. Coccia, D. Lopez Duran, E. Bodo, F. A. Gianturco: J. Phys. Chem. A **111** (2007), 12289, *Microsolvation of Cationic Dimers in ^{4}He Droplets: Geometries of $A_2^+(He)_N$ (A = Li, Na, K) from Optimized Energies*

2. E. Coccia, E. Bodo, F. Marinetti, F. A. Gianturco, E. Yurtsever, M. Yurtsever, E. Yildirim: J. Chem. Phys. **126** (2007), 124319, *Bosonic helium droplets with cationic impurities: Onset of electrostriction and snowball effects from quantum calculations*

1. F. Marinetti, E. Coccia, E. Bodo, F. A. Gianturco, E. Yurtsever, M. Yurtsever, E. Yildirim: Theo. Chem. Acc. **118** (2007), 53, *Bosonic helium clusters doped by alkali metal cations: interaction forces and analysis of their most stable structures*

Scientific communications

5 invited talks and 11 seminars, 20 oral communications and 17 posters in conferences.

Invited talks

Feb 2019	"WaveT/TDPlas: stochastic Schrödinger equation, parallelization and tools" at the "ERC TAME Plasmons Coding Workshop" in Venice (Italy)
May 2017	"Quantum Monte Carlo for electronic structure: excited-state calculations using linear response theory" at the Workshop on "Theory and applications of RPA-and-beyond methods in physics and chemistry" in Paris (France)
Sep 2016	"Quantum Monte Carlo methods for excited states" at the MESBA 2016 Meeting in Buenos Aires (Argentina)
Nov 2014	"Correlated methods for optical properties of pigments: the case of the peridinin" at the "Jam session in photosynthesis: bridging the gap between experimental and theoretical spectroscopy", Amsterdam (The Netherlands)
Jun 2013	"Accurate quantum chemistry calculations for chromophores in photoactive proteins" at the PRACE Scientific Conference in Leipzig (Germany)

Seminars

Jun 2018	"Coherence in ultrafast processes: from single molecule to plasmonic nanostructures" at the Laboratoire de Chimie Theorique - Sorbonne Universites, Paris (France)
Oct 2017	"How the environment affects the optical response of a molecule? Application to nanoparticle-chromophore systems and to fluorophores" as Nano Colloquia at the S3 CNR center, Modena (Italy)
Sep 2017	"Theoretical approaches for electronic and optical properties of metal nanoparticle-molecule systems, fluorophores and biochromophores" at the Dipartimento di Scienze Chimiche, Universitá di Padova, Padova (Italy)
Mar 2017	"Ground- and excited-state properties in theoretical quantum chemistry: stochastic models and approximations from atoms to biochromophores" at the Dipartimento di Chimica, "Sapienza" Universitá di Roma
Nov 2016	"Quantum chemistry and spectroscopy: models and approximations from atoms to biochromophores" at the Dipartimento di Scienze Fisiche e Chimiche, Universitá dell'Aquila, L'Aquila (Italy)
Apr 2016	"Time-dependent quantum chemistry for high-harmonic generation spectroscopy" at the S3 CNR center, Modena (Italy)
Sep 2015	"The Jastrow Antisymmetrized Geminal Power ansatz in chemistry: quantum Monte Carlo developments and applications" at the LPCP, Université Paul Sabatier, Toulouse (France)
May 2015	"Time-dependent configuration interaction for high-harmonic generation: theory and applications" at the Laboratoire Jacques-Louis Lions, Université Pierre et Marie Curie, Paris (France)
Oct 2014	"Quantum Monte Carlo geometry optimization of chromophores of biological interest" at the Department of Physics, Universidad de Chile, Santiago of Chile (Chile)
May 2014	"Quantum Monte Carlo geometry optimization of large molecules: the JAGP ansatz applied to chromophores of biological interest" at the Laboratoire de Chimie Théorique, Université Pierre et Marie Curie, Paris (France)
Dec 2009	"Chemical solutions in a Quantum Solvent: a study of doped Helium clusters" at the Faculty of Engineering, University of L'Aquila, L'Aquila (Italy)

Oral presentations

Sep 2019	"Vibrational coherence in two-pulse ultrafast spectroscopy on single molecule" at the "VI Congresso della Divisione di Chimica Teorica e Computazionale" in Arcavacata di Rende (Italy)
Sep 2018	"Wave function-based approach to probe coherence in ultrafast molecular processes" at the "V Congresso della Divisione di Chimica Teorica a Computazionale" in Trieste (Italy)
Jun 2018	"Probing coherence in ultrafast photoinduced processes: a quantum chemistry perspective" at the PPES18 Conference in Pisa (Italy)

May 2018	"Probing coherence in ultrafast molecular processes: a theoretical perspective" at the "Conference on the Complex Interactions of Light and Biological Matter: Experiments meet Theory" in Trieste (Italy)
Mar 2018	"Quantum coherence in ultrafast molecular processes: ab initio simulations including dephasing" at the 255th ACS National Meeting in New Orleans (USA)
Feb 2018	"Quantumness in ultrafast molecular processes: a Quantum Chemistry approach" at the Quantum Tea @ DiSC for Quantum Technologies in Padova (Italy)
Feb 2018	"Probing quantum coherence in ultrafast molecular processes: an ab initio approach to open quantum systems" at the Winter College on Extreme Non-linear Optics, Attosecond Science and High-field Physics in Trieste (Italy) (flash presentation)
Aug 2017	"Relaxation and dephasing for molecules close to plasmonic nanoparticles: an ab initio approach" at the WATOC 2017 in Munich (Germany)
Jul 2017	"Relaxation and dephasing for molecules close to plasmonic nanoparticles: an ab initio approach" at the Plasmonica 2017 Meeting in Lecce (Italy)
May 2016	"Time-dependent quantum chemistry for high-harmonic generation spectroscopy" at the GDR REST Meeting in Roscoff (France)
Jul 2015	"On the efficiency of Gaussian continuum basis for high-harmonic generation within time-dependent configuration interaction" at the CHITEL 2015 in Turin (Italy)
Jul 2015	"Time-dependent configuration interaction for high-harmonic generation" at the GDR Correl Meeting in Marseille (France)
Jun 2015	"High-harmonic generation for the hydrogen atom using time-dependent configuration interaction" at the 12^{th} ETSF Young Researchers' Meeting in Paris (France)
May 2014	"Interplay between geometry and optical properties in biological chromophores: Quantum Monte Carlo ground state structures for RPSB and peridinin molecules" at the 11^{th} ETSF Young Researchers' Meeting in Rome (Italy)
Mar 2014	"Quantum Monte Carlo and Many Body Green's Function Theory Calculations for Biological Chromophores" at the Winter Modeling 2014 workshop in Modena (Italy)
Sep 2013	" QMC and quantum chemistry calculations for chromophores in photoactive proteins" at the EuCo-CC9 conference in Sopron (Hungary)
Feb 2013	"Protein field effect on the dark state of 11-*cis* Retinal in Rhodopsin by Quantum Monte Carlo/Molecular Mechanics" at the II Congresso DCTC in Padova (Italy)
Jun 2012	"Quantum Monte Carlo/Molecular Mechanics: geometry optimization of the Retinal chromophore in gas phase and in Rhodopsin" at the TUMA 2012 conference in Francavilla al Mare (L'Aquila, Italy)
Mar 2012	"Quantum Monte Carlo/Molecular Mechanics: relaxed geometries of Retinal in gas phase and in Rhodopsin" at the *New QM/MM opportunities for in silico macromolecular spectroscopy* in Lyon (France)
Jun 2010	"Understanding vibrational motions in molecular systems: quantum mechanics (QM), molecular mechanics (MM) and "mixed" QM/MM approaches in chemistry" at the *Giornata di Incontro Universitá-Aziende del Territorio Aquilano sulla Chimica e Scienza dei Materiali* in L'Aquila (Italy)

Posters

Feb 2018	"Probing quantum coherence in ultrafast molecular processes: an ab initio approach to open quantum systems" at the Winter College on Extreme Non-linear Optics, Attosecond Science and High-field Physics in Trieste (Italy)
Apr 2017	"Real-time electronic propagation with dissipation and dephasing: the LiCN molecule close to a metal nanoparticle" a the Molecular properties and Computational Spectroscopy meeting in Pisa (Italy)
Jan 2017	"TAME-Plasmons: a Theoretical Chemistry Approach to Time-Resolved Molecular Plasmonics" at the Italian ERC Chem Day in Rome (Italy)
Jan 2017	"Langevin equation and quantum Monte Carlo: a study of the rotational states of doped ^{4}He clusters" at the GLE2017 workshop in London (UK)
Jun 2015	"High-harmonic generation within time-dependent configuration interaction" at the Labex MiChem International Symposium in Paris (France)
Oct 2013	"Ab initio geometry and bright excitation of carotenoids: Quantum Monte Carlo and Many Body Green's Function Theory calculations on peridinin" at the Biophysics of Photosynthesis (BIOPHROME2013) Conference in Rome (Italy)
Jan 2013	"Protein Field Effect on the Dark State of 11-*cis* Retinal in Rhodopsin by Quantum Monte Carlo/Molecular Mechanics" at the Total Energy conference in Trieste (Italy)
Sep 2011	"Quantum Monte Carlo methods for molecular polarizabilities within a hybrid QMC/MM scheme" at the CPMD2011 conference in Barcelona (Spain)
Sep 2010	"Influence of effective normal modes on electronic excitations: QM/MM simulations of acetone in different solvents" at the Ψ_k 2010 conference in Berlin (Germany)
Oct 2009	"The $Cs_2(^3\Sigma_u)$-He complex as a weakly bound species" at the *Efimov states in molecules and nuclei: Theoretical methods and new experiments* in Rome (Italy)
May 2009	"Light diatomic molecules in ^{4}He clusters: a Quantum Monte Carlo approach" at the QFC09 conference in Dresden (Germany)
Aug 2008	"Chemical solutions in a quantum solvent: anionic electrolytes in ^{4}He nanodroplets" at the MOLEC XVII conference in St. Petersburg (Russia)
Jul 2008	"Impurezze atomiche e molecolari in gocce di ^{4}He: applicazione dei metodi Quantum Monte Carlo ai sistemi a molti corpi" at the *III Convegno Giovani Chimici* in Rome (Italy)
Jan 2008	"Anionic dopants in ^{4}He nanodroplets: $OH^-(He)_N$ structures from quantum Monte Carlo calculations" at the MiniWorkshop on QMC methods in Trieste (Italy)
Oct 2007	"Quantum structuring and microenergetics of ionic dopants in ^{4}He droplets from stochastic calculations" at the *Molecular and nanodynamics: from atoms to biomolecules* conference in Rome (Italy)
May 2007	"Quantum structuring and microenergetics of ionic dopants in ^{4}He droplets from stochastic calculations" at the ECAMP IX conference in Heraklion (Greece)
Mar 2005	"Interaction of p-H_2 with ^{4}He atoms: A quantum Monte Carlo analysis" at the *343rd WE-Heraeus-Seminar on helium nanodroplets* in Bad Honnef (Germany)

Visiting

- Jun 2018: Laboratoire de Chimie Theorique - Sorbonne Universites, Paris (France)
- Jun 2015: The Head-Gordon group Berkeley - University of California, Berkeley (USA)

Visitors

- Jan-Apr 2019: Zelipe Zapata-Abellan (PhD Student at Sorbonne University)

Teaching

- 2019-: "Tecniche di programmazione in chimica computazionale (Programming in computational chemistry)", University of Trieste, Italy
- 2015: ICS Summer School "*Introduction to Quantum Monte Carlo*", UPMC, France
- 2013-2014: "General Chemistry", University of L'Aquila, Italy
- 2012: Mini-course within the MathMods Programme in Mathematical Models in Life and Social Sciences "*Introduction to Linux*", University of L'Aquila, Italy
- 2012: "*Esercitazioni di Chimica*", University of L'Aquila, Italy
- 2011: Mini-course within the MathMods Programme in Mathematical Models in Life and Social Sciences "*Introduction to Linux*", University of L'Aquila, Italy
- 2010: Mini-course within the MathMods Programme in Mathematical Models in Life and Social Sciences "*The Monte Carlo theory in physics and chemistry*", University of L'Aquila, Italy

Theses

- Coadvisor of the Master Thesis in Mathematical Modelling in Engineering "Molecular modeling of the excitation energy transfer in Photosystem II" by Marco Manzoli (2013).
- Coadvisor of the Master Thesis in Mathematical Modelling in Engineering "Finding Minimum Energy Paths on Error-Affected Potential Energy Surfaces" by Miriam Garcia Soto (2012).
- Coadvisor of the Master Thesis in Mathematical Modelling in Engineering "Electronic Density Estimator by Quantum Monte Carlo" by Olga Chernomor (2011).

Grants awarded

Principal Investigator

- Apr 16, 2019 - : 30,400,000 core hours on SuperMUC HPC computer - Germany (PRACE Project "NANOMOLEL - Antenna-reactor nanostructures for electron injection in molecules")

- Feb 7, 2019-: 35,000 core hours on Marconi HPC cluster - Italy (ISCRA C Project "Vibronic coherence in ultrafast spectroscopy: a molecular study using stochastic methods")
- Feb 1, 2018 - Aug 2, 2018 : 200,000 core hours on Curie HPC cluster - France (Preparatory access Prace Tier0 Project of Type B: "Probing environmental effects for ultrafast spectroscopy of molecules using stochastic Schroedinger equation and quantum chemistry")
- May 10, 2017- Feb 10, 2018 : 15,000 core hours on Marconi HPC cluster - Italy (ISCRA-C Project "Dissipation and dephasing for molecules close to plasmonic nanoparticles: an ab initio approach")
- Jul 21, 2017-Apr 30, 2018 : 2,170,467 core hours on Archer HPC cluster - UK (DECI-13 Project "QMCPHE: π-interactions in the Phenalenyl dimer and in its derivatives through quantum Monte Carlo and the Jastrow Antisymmetrized Geminal Power ansatz")
- Jul 21, 2016-May 21, 2017: 50,000 core hours on Marconi HPC cluster - Italy (ISCRA C Project "SP-QMC: Spin polarization and quantum Monte Carlo: insights from the Jastrow Antisymmetrized Geminal Power ansatz")
- Nov 15, 2014-Nov 15, 2015: 5,000 Euro from the LabEx MiChem part of French state funds managed by the ANR within the Investissements d'Avenir programme under reference ANR-11-IDEX-0004-02
- Mar 15, 2013-Mar 15, 2014: 950,000 core hours on FERMI HPC cluster - Italy (ISCRA B Project "QMC-poly: Quantum Monte Carlo polarizability of long polyacetylene chains")
- May 2, 2013-May 15, 2014: 40,000 core hours on Europa/PLX cluster - Italy (ISCRA B project 'QMC-poly: Quantum Monte Carlo polarizability of long polyacetylene chains")
- Oct 31, 2012-Oct 31, 2013: 1,000,000 core hours on FERMI HPC cluster - Italy (ISCRA B Project "RHOD-QMC: Rhodopsin environmental effects on the Retinal ground state structure: a Quantum Monte Carlo study")
- Dec 15, 2011-Apr 15, 2013: 600,000 core hours on FERMI HPC cluster - Italy (ISCRA B Project "MolQMC: Fully Correlated Molecular Electric Properties by Quantum Monte Carlo")

Collaborator

- Apr 3, 2017-: 5,225,000 core hours on Marconi HPC cluster - Italy (Prace Tier0 Project: "Novel synthesis Routes for carbon based 1D nanoMaterials")
- Mar 14, 2016-Mar 13, 2017: 4,000,000 core hours on FERMI HPC cluster - Italy and 737,268 core hours on Marconi HPC cluster (Prace Tier0 Project: "EyESPOT Electronic states in pure and doped rutile and anatase TiO2")
- Sep, 1 2014-Sep, 1 2015: 45,420,000 core hours on JUQUEEN HCP cluster - Germany (Prace Tier0 Project: "BIOCHROMO - Ground state structures and electronic excitations of biological chromophores at Quantum Monte Carlo / Many Body Green's Function Theory level")
- Sep 3, 2013-Sep 2, 2014: 9,200,000 core hours on FERMI HPC cluster - Italy (Prace Tier0 Project: "MODYQA - Molecular dynamics simulation of liquid water by quantum Monte Carlo")
- Sep 3, 2013-Sep 3, 2014: 6,508,160 core hours Curie HPC cluster - France (Prace Tier0 Project: "PHOTOSYSTEM2 - Water oxidation by photosynthesis: dynamics and reactivity of the manganese cluster in the Photosystem II complex explored by Quantum Mechanics / Molecular Mechanics simulations")

- Mar 1, 2013-Feb, 28 2014: 38,990,000 core hours on Juqueen HPC cluster - Germany (Prace Tier0 Project: "RHODQMC - Energy storage in the first step of vision explored by Quantum Monte Carlo / Molecular Mechanics calculations")
- Mar 15, 2013-Mar 15, 2014: 920,000 core hours on FERMI HPC cluster - Italy (ISCRA B Project: "QMMMPSII")
- Nov, 1 2011- Aug, 31 2012: 44,564,480 on JUGENE HPC cluster - Germany (Prace Tier0 Project: "Protein effects on the structural and optical properties of biological chromophores: Quantum Monte Carlo / Molecular Mechanics calculations on Rhodopsin and Light Harvesting Complexes")
- Jun 21, 2011-Jan 21, 2013: 150,000 core hours on FERMI HPC cluster - Italy (ISCRA B Project: "ENVELOP")
- Jun 21, 2011-Nov 21, 2012: 150,000 core hours on FERMI HPC cluster - Italy (ISCRA B Project: "QMC-BLA")
- Jul 19, 2010-Sep 19, 2011: 600,000 core hours on SP cluster - Italy (ISCRA A Project: "LQW")
- Jul 19, 2010-Jul 19, 2011: 100,000 core hours on FERMI HPC cluster - Italy (ISCRA B Project: "SPLITH20")
- Jul 7, 2011-Dec 31, 2011: 250,000 on JUGENE HPC cluster - Germany and 200,000 core hours on Curie HPC cluster -France (Preparatory access Prace Tier0 Project: "Quantum Monte Carlo methods for biological systems")

Reviews

- Reviewer on the Journal of Chemical Theory and Computation, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, Physical Chemistry Chemical Physics, Computational and Theoretical Chemistry, The European Physical Journal Plus
- Reviewer for CINECA ISCRA projects

Technical skills

Excellent experience in

- Linux and OSX operating systems
- Fortran coding
- Parallel (MPI and OpenMP) coding
- Script coding

Good experience in

- C coding
- Python
- GPU/CUDA coding

Other

- Sep 2019: Jury Member for PhD final exam (Theoretical Chemistry), candidate: Felipe Zapata-Abellan (Sorbonne University)
- Jul 2019: Jury Member for PhD final exam (Mathematics and models), candidates: Venanzio di Giulio and Giovanna Rogati (University of L'Aquila)
- Jun 2013: Local organizer of the Summer School on ab initio Molecular Dynamics for Biomolecules in S. Stefano di Sessanio (L'Aquila, Italy)

Trieste, September 23, 2019