Curriculum Vitæ

Francesco Segatta

Personal Information

Name: Francesco Segatta
Citizenship: Italian
Date and Place of Birth: November 25th 1989, Trento, Italy

Contact Information

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Current Position

RTD-A (Research Associate) 2023 - present
Dipartimento di Chimica Industriale "Toso Montanari", University of Bologna

Education

Ph.D. in Chemistry, excellent cum laude 2018
University of Bologna (Unibo) - Fondazione Bruno Kessler (FBK), Italy
Modeling photoinduced events and nonlinear spectroscopy in complex multichromophoric systems
Supervisors: Prof. Marco Garavelli (Unibo) and Dr. Simone Taioli (FBK)

Master's degree in Physics, 110/110, summa cum laude 2014
Department of Physics, University of Trento (Unitn), Italy
A mesoscopic model of charge transport in organic semiconductors
Supervisor: Prof. Pietro Faccioli (Unitn)

Bachelor's degree in Physics, 110/110, summa cum laude 2011
Department of Physics, University of Trento (Unitn), Italy
A simple example of effective theories: how to renormalize the Schrödinger equation
Supervisor: Prof. Marco C. Traini (Unitn)

Research Experience

PostDoctoral Researcher - 4 years 2018 - 2022
Dipartimento di Chimica Industriale "Toso Montanari", University of Bologna
Theory and simulation of ultrafast multidimensional nonlinear X-ray spectroscopy of molecules

PostDoctoral Researcher - 3 months 2020
Prof. David F. Coker's group, *Boston University (BU), Boston, MA, USA*
Energy transfer pathways and mechanisms for photosynthetic light harvesting from 2D electronic spectroscopy and first principles calculations

Visiting Researcher - 5 months 2017
Prof. David F. Coker's group, *Boston University (BU), Boston, MA, USA*
Partial linearized density matrix & nonlinear spectroscopy simulation

Research training fellowship - 1 month 2014
SISSA (Scuola Internazionale Superiore di Studi Avanzati), Trieste, Italy
Sampling polymeric chains conformations with Monte Carlo methods

Teaching Activity

Teaching assistant at Unibo, Corso di "Matematica con Esercitazioni", Faenza, Italy 2019-22
Analysis (one and multiple variables) and Linear Algebra (30 hours/year, totaling 120 hours)

Individual tutoring activity (**Linear Algebra**), *Camp1us College,* Bologna, Italy 2018-19

Individual tutoring activity (**Math and Physics to high school students**), *Scholé,* Bologna & *Associazione Periscopio*, Trento, Italy 2015-17 2009-14

Mentoring Activity

Supervisor of A. Loreti's Master Thesis (Dipartimento di Chimica Industriale, Unibo) 2022
Development of cheaper methods for linear and transient absorption spectroscopy

Supervisor of S. Cauzzi's Bachelor Thesis (Dipartimento di Chimica Industriale, Unibo) 2022
Strategie per individuare la correlazione tra geometria molecolare ed energia di eccitazione

Supervisor of S. Cauzzi's Bachelor Thesis (Dipartimento di Chimica Industriale, Unibo) 2022
Simulazione di spettroscopia di assorbimento a raggi X della molecola Idrossiclorochina

Supervisor of F. Montorsi's Master Thesis (Dipartimento di Chimica Industriale, Unibo) 2022
Transient X-ray spectroscopy to unravel photo-induced processes in molecular systems

Supervisor of M. Wauters's Bachelor Thesis (Unibo - UCLL Belgium) 2021
Simulation of linear absorption and photoelectron spectroscopy of the thymine molecule

Supervisor of F. Montorsi's Bachelor Thesis (Dipartimento di Chimica Industriale, Unibo) 2020
Simulazione computazionale di spettroscopia NEXAFS transiente di dinamiche fotoindotte

Co - Supervisor of G. Biffi's Master Thesis (Dipartimento di Chimica, Unibo) 2018
Excitonic model for simulations of molecular crystals electronic spectroscopy

Peer-Rev. & Editorial Activity

Member of the editorial board (as Review Editor) for **Computational Materials Science** (Frontiers in Materials)

Referee for **Journal of Physical Chemistry Letters**, **Physical Chemistry Chemical Physics**, **Journal of Chemical Theory and Computation, Molecules** *(MDPI)*, **Chemical Physics Letters**

Bibliometric Indexes*

Number of documents: 25[a] (25)[b]
Number of citations: 610 (774)
H - index: 12 (12)

[a] Source: *Scopus* [b] Source: *Google Scholar*
* Updated to Sept. 2023

Honours & Awards

National Scientific Qualification as associate in the Italian higher education system 2023

Eolo Scrocco Prize, Divisione di Chimica teorica - Società Chimica Italiana (SCI) 2022
https://www.soc.chim.it/it/divisioni/teocomp/premi

Best Poster Prize at the ISTCP-X conference (12 prizes/300 posters), Tromsø, Norway 2019

Certificate of Excellence - FBK International PhD program award, Trento, Italy 2019

Best group project, *SMART* Winter School, *Scuola Normale Superiore* (SNS), Pisa, Italy 2016

Master degree award at University of Trento, Trento, Italy 2014

Funds[§]

PostDoc funding: U.S. Department of Energy, Office of Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division under Award No. DE-SC0019484 & DE-SC0019484 (78,000 €) — 2018 - 2022

Project titles: Theory and Simulation of Ultrafast Multidimensional Nonlinear X-ray Spectroscopy of Molecules; Modeling of Multidimensional X-ray Probes of Chemical Processes and Dynamics in Molecular Systems

Project PIs: Shaul Mukamel (UCI, lead PI), Sergei Tretiak (LANL, Co-PI), Niranjan Govind (PNNL, Co-PI), Marco Garavelli (Unibo, Co-PI)

PostDoc funding: U.S. Department of Energy, Office of Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division under Award No. DE-SC0020437 (10,500 $, net amount) — 2020

Project title: Energy Transfer Pathways and Mechanisms for Photosynthetic Light Harvesting from 2D Electronic Spectroscopy and First Principles Calculations

Project PIs: David F. Coker (BU, lead PI), Ksenia Bravaya (BU, Co-PI), Sahar Sharifzadeh (BU, Co-PI), Gregory D. Scholes (Unibo, Co-PI)

PhD Mobility funding: Marco Polo Mobility Fellowship, Awarded by the Unibo Department of Chemistry G. Ciamician (3,000 €, net amount) — 2017

Project title: Multi-Chromophoric Systems: Exciton Dynamics in Complex Environments

Supervisor(s): Prof. David F. Coker (Boston University, Boston, MA, USA), Prof. Marco Garavelli (Unibo)

PhD fellowship funding: Fondazione Bruno Kessler (FBK - Trento) (49,000 €) — 2014 - 2017

Project title: Modeling photo-induced events and nonlinear spectroscopy in complex multichromophoric systems

Supervisor(s): Prof. Marco Garavelli (Unibo), Dr. Simone Taioli (FBK)

Training fellowship funding: Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste (1,000 €, net amount) — 2014

Project title: Sampling polymeric chains conformations with Monte Carlo methods

Supervisor: Prof. Cristian Micheletti

[§] Gross amount, unless otherwise stated

Computer Skills

Good command of the Operating Systems: *MacOS, Linux, Windows*

Good command of the programming languages: *C/C++, Fortran, Python, Matlab, bash, latex*

Good command of the computational Chemistry Software: *Molcas/OpenMolcas, Gaussian, Molden, Spectron* (co - developer)

Good command of the graphical tools: *gnuplot, OrbKit, VMD, Origin*

Developer of the iSPECTRON interface (https://github.com/ispectrongit/iSPECTRON)

Voluntary Work

Organizer of fundraising events for the NPOs: *EDUS, AVSI, Banco Alimentare*

Languages

English: advanced (C1 level)

Italian: native

Conferences & Seminars

Oral presentation at *FEMTO15, Berlin, Germany* 2023
Simulation of molecular electronic spectroscopy via (MCTDH) quantum dynamics: from exact to approximate expressions

Invited Oral presentation at the *SLAC National accelerator laboratory Photon Science Seminar Series,* given online 2022
Accurate Ab-initio Soft X-ray Spectroscopy Simulation of Molecules: Method, Examples and Insight

Invited Oral presentation at *WATOC-2020,* Vancouver, Canada 2022
A Gentle Introduction to X-ray Photoelectron Spectroscopy of Molecular Systems

Poster presentation to *WATOC-2020,* Vancouver, Canada 2022
Simulation of Linear and Nonlinear X-ray Spectroscopy: Basics, Tools and Examples

Oral presentation to ETSF-25^{th} *Workshop on Electronic Excitations,* Leuven, Belgium 2022
Core-level Spectroscopy of Molecules with Multiconfigurational Wave-function Theory

Oral presentation to 10^{th} *OpenMolcas Developers' Meeting,* Uppsala, Sweden 2022
Core-level excitation and ionization with OpenMolcas: Spectrum Completeness, Quantitative Reproduction of Line Shapes, and Physical Insight

Oral presentation and Session Host to *The International Chemical Congress of Pacific Basin Societies 2021 (PACIFICHEM)* 2021
Simulation of X-ray linear and nonlinear spectroscopy of the ESCA molecule

Poster presentation to *Time Resolved Vibrational Spectroscopy (TRVS2021)* 2021
Visualizing molecular vibrations via ultrafast UV-pump (soft) X-ray probe spectroscopy; Theory and Experiment

Oral presentation to 8^{th} *OpenMolcas Developers' e-Meeting* 2020
Simulation of X-ray linear and nonlinear spectroscopy with OpenMolcas

Oral presentation to *Quantum Effects in Complex Systems* - Faraday Discussion Coventry, United Kingdom 2019
Exploring the capabilities of optical-pump X-ray probe NEXAFS spectroscopy to track photoinduced dynamics mediated by conical intersections

Poster presentation to ISTCP-X, Tromsø, Norway 2019
Simulation of optical-pump X-ray probe NEXAFS spectroscopy to track photoinduced dynamics of organic molecules

Oral presentation to *WINTER MODELING*, Napoli, Italy 2019
Ultrafast carotenoid to retinal energy transfer in Xanthorhodopsin revealed by two dimensional electronic spectroscopy

Oral presentation to *FBK-PhD DAY*, Trento, Italy 2018
Modeling quantum properties and nonlinear spectroscopy in complex systems of interacting molecules

Poster presentation to *WATOC 2017*, Munich, Germany 2017
Modeling photoinduced events and nonlinear spectroscopy in complex multichromophoric systems

Poster presentation to *ACTC*, Boston, MA, USA 2017
Modeling photoinduced events and nonlinear spectroscopy in complex multichromophoric systems

Oral presentation to *Enlight Workshop*, Pisa, Italy 2016
Linear/nonlinear spectroscopy in LH2 within a first principle Frenkel Exciton model

Oral contribution to the first "*Assemblea del Dipartimento di Fisica*", Trento, Italy 2015
I corsi di studio in Fisica

Research Activity

Francesco Segatta

My research activity has been mainly devoted to the development and application of theoretical/computational methods in two fields, namely: **computational quantum chemistry** and **spectroscopy simulation** of molecular and super-molecular systems.

Computational Quantum Chemistry: in this field, under the mentorship of Prof. Marco Garavelli and the collaboration with the members of His research group, I learnt the nuances of multiconfiguration wavefunction-based ab-initio approaches to solve the time-independent Schrödinger equation, such as the complete active space self consistent field (CASSCF/CASPT2). The CASSCF/CASPT2 approach represents the state-of-the-art for its accuracy in the description of excited states of generic small/medium size molecular systems, and recent developments suggest it can be also applied to larger photo-responsive molecular materials.
Along my past and present research activity, I developed approaches to extend the applicability of these methods, introducing original contributions to treat: the intermolecular couplings in large multichromophore systems (*cf.* papers 4, 9, 11, 12, 14), the dynamical interaction between photoactive molecules and solvent (*cf.* papers 2, 7), and the computation of core-level excitations (*cf.* papers 1, 6, 8, 15-19). More recently, the collaboration with Prof. Niranjan Govind (Pacific Northwest National Laboratory, Richland, USA) has also exposed me to TDDFT type calculations, to describe both valence and core-level excitations (*cf.* papers 2-3, 8).

Simulation of Spectroscopy: in the research activity conducted so far, the accurate quantum chemical description of molecular systems (being them an isolated molecule or a molecular aggregate, in gas-phase or in complex environments), has always been coupled to the study of its response to light induced perturbations, i.e., the simulation of spectroscopy. The Response Function approach, developed by Prof. Shaul Mukamel (which I collaborate with), has been the powerful theoretical tool to describe linear, as well as coherent multidimensional nonlinear time-resolved spectroscopic techniques (such as transient absorption, and two-dimensional electronic spectroscopy), from the VIS/UV to the X-ray. I applied this approach to a large variety of systems (LH2 of rps. acidophila, xanthorhodopsin, azobenzene, pyrene, etc.) reproducing experimental spectra and fostering their interpretation, while producing unprecedented insight into their photophysical and photochemical properties (*cf.* papers 1-2, 4, 6-8, 11-12, 14-18, 23).

The expertise that I acquired over the years, by conducting research in both of these above mentioned areas, and by collaborating with world leading experimental groups (Prof. Giulio Cerullo, Polimi, Milano; Prof. Claudio Masciovecchio, Elettra Synchrotron, Trieste), has allowed me to develop a unique understanding of light-matter interaction in molecular and supra-molecular systems. I introduced original contributions in both fields, as, e.g.: the development of a semiclassical path integral approach for the calculation of linear and nonlinear optical spectroscopy (during a visiting period in the research group of Prof. David Coker at Boston University) and its recent extension to explicitly account for the field properties (*cf.* papers 5, 13); the quantum dynamics based simulation of nonlinear spectroscopy (in collaboration with Prof. Fabrizio Santoro, CNR-Pisa); the characterization of spectral line-shape impact of solvent-solute interaction (*cf.* paper 7); the study of the information content of X-ray spectroscopic techniques with unparalleled insight (*cf.* papers 1, 6, 8, 16-19). Eventually, I also developed and published a software (iSPECTRON) that facilitates the path from quantum chemistry to spectra (*cf.* paper 3).

List of Publications

Francesco Segatta

List updated to October 2022 † *First author(s), * corresponding author(s)*

Publications as first author / corresponding author

1. Montorsi F.,[†] Segatta F.,[*] Nenov A., Mukamel S., Garavelli M.,[*] **Soft X-ray Spectroscopy Simulations with Multiconfigurational Wave Function Theory: Spectrum Completeness, Sub-eV Accuracy, and Quantitative Reproduction of Line Shapes**, *J. Chem. Theory Comput., 18(2),* (2022)

2. Segatta F.,[†*] Russo M., Nascimento R. D., Presti D., Rigodanza F., Nenov A., Bonvicini A., Arcioni A., Mukamel S., Maiuri M., Muccioli L., Govind N.,[*] Cerullo G.,[*] Garavelli M.,[*] **In silico ultrafast nonlinear spectroscopy meets experiments: the case of perylene bisimide dye**, *J. Chem. Theory Comput., 17(11),* (2021)

3. Segatta F.,[†] Nenov A., Nascimento D. R., Govind N.,[*] Mukamel S.,[*] Garavelli M.,[*] **iSPECTRON: A Simulation Interface for Linear and Nonlinear Spectra with ab-initio Quantum Chemistry Software**, *J. Comput. Chem.*, 42(9), 644 (2021)

4. Segatta F.,[†] Rogers D. M., Dyer N. T., Guest E. E., Li Z., Do H. Nenov A., Garavelli M., Hirst J. D.,[*] **Near-Ultraviolet Circular Dichroism and Two-Dimensional Spectroscopy of Polypeptides**, Molecules, 26(2), 396 (2021)

5. Provazza J.,[†] Segatta F.,[†] Coker D. F.,[*] **Modeling nonperturbative field-driven vibronic dynamics: Selective state preparation and nonlinear spectroscopy**, *J. Chem. Theory Comput.*, 17(1), 29 (2020)

6. Segatta F.,[†] Nenov A.,[†] Orlandi S., Arcioni A., Mukamel S., Garavelli M.,[*] **Exploring the Capabilities of optical-pump X-ray probe NEXAFS Spectroscopy to Track Photo-indued Dynamics Mediated by Conical Intersections**, *Faraday Discuss.*, 221, 245 (2019)

7. Segarra-Martí J.,[†*] Segatta F.,[†*] Mackenzie T. A., Nenov A.,[*] Rivalta I., Bearpark M. J., Garavelli M., **Modeling Multidimensional Spectral Lineshapes from First Principles: Application to Water-Solvated Adenine**, *Faraday Discuss.*, 221, 219 (2019)

8. Nenov A.,[†] Segatta F.,[†] Bruner A.,[†] Mukamel S., Garavelli M.,[*] **X-ray Linear and Nonlinear Spectroscopy of the ESCA molecule**, *J. Chem. Phys.*, 151(11), (2019)

9. Segatta F.,[†] Capellini L.,[†] Garavelli M.,[*] Mennucci B.,[*] **Quantum Chemical Modeling of the Photoinduced Activity of Multichromoporic Biosystems**, *Chem. Rev.*, 119(16), 9361 (2019)

10. Segatta F.,[†] Lattanzi G., Faccioli P.,[*] **Predicting Charge Mobility of Organic Semiconductors with Complex Morphology**, *Macromolecules*, 51(21), 9060 (2018)

11. Segatta F.,[†] Gdor I., Réhault G., Taioli S., Friedman N., Sheves M., Rivalta I., Ruhman S.,[*] Cerullo G.,[*] Garavelli M.,[*] **Ultrafast Carotenoid to Retinal Energy Transfer in Xanthorhodopsin Revealed by the Combination of Transient Absorption and Two Dimensional Electronic Spectroscopy**, *Chem.-Eur. J.*, 24(46), 12084 (2018)

12. Segatta F., **Modeling Photoinduced Events and Nonlinear Spectroscopy in Complex Multichromophoric Systems**, Phd Thesis, http://amsdottorato.unibo.it/8469/ (2018)

13. Provazza J.,[†] Segatta F.,[†] Garavelli M., Coker D. F.,[*] **Semiclassical Path Integral Calculation of Nonlinear Optical Spectroscopy**, *J. Chem. Theory Comput.*, 14(2), 856 (2018)

14. Segatta F.,[†] Cupellini L., Jurinovich S., Mukamel S., Dapor M., Taioli S., Garavelli M.[*] and Mennucci B.,[*] **A Quantum Chemical Interpretation of Two-Dimensional Electronic Spectroscopy of Light-Harvesting Complexes**, *J. Am. Chem. Soc.*, 139(22), 7558 (2017)

Other publications

15. Nam Y.,[†*] Keefer D., Nenov A., Aleotti F., Conti I., Segatta F., Yong Lee J.,[*] Garavelli M., Mukamel S.,[*] **Conical Intersection Passages of Molecules Probed by X-ray Diffraction and Stimulated Raman Spectroscopy**, *J. Phys. Chem. Lett., 12(51),* (2021)

16. Keefer D.,[†] Rouxel R. J., Aleotti F., Segatta F., Garavelli M., Mukamel S.,[*] **Diffractive Imaging of Conical Intersections Amplified by Resonant Infrared Fields**, *J. Am. Chem. Soc., 143(34),* (2021)

17. Cavaletto S. M.,[†] Keefer D., Rouxel J. R., Aleotti F., Segatta F., Garavelli M., Mukamel S.,[*] **Unveiling the spatial distribution of molecular coherences at conical intersections by covariance X-ray diffraction signals**, *P. Natl. Acad. Sci. USA*, 118(22), (2021)

18. Keefer D.,[†] Aleotti F., Rouxel J. R., Segatta F., Gu B., Nenov A., Garavelli M., Mukamel S.,[*] **Imaging conical intersection dynamics during azobenzene photoisomerization by ultrafast X-ray diffraction**, *P. Natl. Acad. Sci. USA*, 118(3), (2021)

19. Gu B.,[†] Nenov A.,[†] Segatta F., Garavelli M.,[*] Mukamel S.,[*] **Manipulating Core Excitations in Molecules by X-Ray Cavities**, *Phys. Rev. Lett.*, 126(5), (2021)

20. Aquilante F., Segatta F., Veryazov V.,[*] *et al*, **Modern Quantum Chemistry with [Open]Molcas**, *J. Chem. Phys.*, 152(21), 214117 (2020)

21. Alvertis A.M., Barford W., Worster S.B., Burghardt I., Datta A., Dijkstra A., Fay T., Ghosh S., Grünbaum T., Habershon S., Hore P.J., Hutchinson D., Iyengar S., Jones A.R., Jones G., Komarova K., Lawrence J., Léonard J., Litman Y., Mannouch J., Manolopoulos D., Martens C., Mondelo-Martell M.,Picconi D., Plant D., Sakaushi K., Saller M.AC., Schile A., Scholes G.D., Segarra-Martí J., Segatta F., Troisi A., Worth G., **Quantum coherence in complex environments: general discussion**, *Faraday Discuss.*, 221, 168 (2019)

22. Alvertis A.M., Barford W., Worster S.B., Burghardt I., Chin A., Datta A., Dijkstra A., Fay T., Fielding H., Grünbaum T., Habershon S., Hammes-Schiffer S., Iyengar S., Jones A.R., Komarova K., Léonard J., Litman Y., Picconi D., Plant D., Schile A., Scholes G.D., Segarra-Martí J., Segatta F., Troisi A., Worth G., **Spectroscopic signatures of quantum effects: general discussion**, *Faraday Discuss.*, 221, 322 (2019)

23. Nenov A.,[†] Borrego-Varillas R.,[†] Oriana A., Ganzer L., Segatta F., Conti I., Segarra-Marti J., Omachi J., Dapor M., Taioli S., Manzoni C., Mukamel S., Cerullo G.,[*] Garavelli M.,[*] **UV-light induced vibrational coherences, the key to understand Kasha rule violation in trans-azobenzene**, *J. Phys. Chem. Lett.*, 9(7), 1534 (2018)