Curriculum vitae et studiorum [1]

of Dr. Fabrizio Santoro

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Google Scholar https://scholar.google.it/citations?user=mGqD66cAAAAJ&hl=it

Place and date of birth: Napoli (Italy), 14/7/1970

- Senior Research Scientist of Italian National Council of Research.
- 2011-2013 Member of the Board of the Theoretical and Computational Chemistry Division of the Italian Chemical Society
- Awarded in 2013 with the National Qualification as Full Professor in Physical Chemistry.
- Associated member of INSTM, the National Institute for Material Science Technologies

H-Index: 32 (ISI), 35 (Google Scholar)

Education

1999: PhD Degree in Chemistry at the Universities of Perugia and of Siena, defending the thesis "$\tilde{X}^2A_1/\tilde{A}^2B_2$ conical intersection effects on the absorption spectrum and the intramolecular dynamics of NO_2".

1994: Master Degree in Chemistry at University "Federico II" of Napoli (110/110 cum laude) with the thesis: "Theoretical study of the electron transfer in biological systems".

1988: Scientific High School Degree (60/60).

Teaching and Training Activity

2015-2016 supervisor at ICCOM-CNR of a one-year secondment of a phD student of Shan Dong University, China, funded by Shan Dong University, PhD Mobility Program

2014-2016 supervisor at ICCOM-CNR of a PostDoc position awarded to J. Cerezo funded by Spanish Fundación Ramón Areces

2014 supervisor at ICCOM-CNR of a PostDoc position awarded to J. Cerezo funded by Italian PRIN Project 2010-2011

2012-2014 supervisor of a Marie Curie PostDoc awarded to F. Avila funded EU People Program, Marie Curie Actions (G.A. no. 246550)

2012-2013 supervisor of J. Cerezo a phD student of University of Murcia for a three month placement at ICCOM-CNR

[1] 26 October 2016

2012 supervisor ICCOM-CNR of M. Segado postDoc within the FIRB Project RBFR10Y5VW "Towards knowledge-based systems for organic photovoltaics"
2011-2012 supervisor of D. Padula for the phD thesis "Structure and Properties of Simple and Aggregate Systems by Circular Dichroism" at University of Pisa

2011-2012 supervisor of D. Picconi for a thesis "Methods for Quantum Dynamics: Application to photoexcited DNA nucleobases", for "Laurea Specialistica" in Chemistry

2011-2012 supervisor of Francisco Avila Ferrer for a 2-year postDoc researcher

2010-teacher of **"**Computational Spectroscopy**"** at Scuola Normale Superiore

2010 supervisor of F. Avila a phD student of Malaga University for a three month placement at IPCF-CNR

2009–2010 supervisor of D. Picconi for the thesis "Ultrafast decay of photoexcited DNA nucleobases", for the Degree in Chemistry

2008-2009 supervisor of Na Lin for a phD thesis "Theoretical Studies on Electronic and Vibrationally Resolved Multi-Photon Absorption and Dichroism" at KTH, Royal Institute of Technology, Stockholm. This thesis has been awarded the best thesis in Theoretical Chemistry in Sweden in 2009

2006–2008 supervisor of D. Paganelli for a thesis "Quantum Dynamics of the Photoisomerization of the protonated Schiff base of Retinal", for the Master Degree in Chemistry

2001 – 2003: professor at the University of Siena (Laboratory of Physical Chemistry III), Degree in Chemistry

1998 – 1999: Professor at the University of Salerno (Molecular Spectroscopy), Degree in Chemistry.

Research Positions in Italy

2007- Senior Research Scientist of the Italian National Council of Research

2001 (21st December)-**2006:**research scientist of the Italian National Council of Research (CNR) at the Istituto per i Processi Chimico-Fisici (IPCF-CNR), in Pisa**.**

2000 – 2001 Post Doc in Physical Chemistry at the University of Siena

1999 – 2000: fellowship at the University of Siena under the supervision of Prof. C. Petrongolo **1995 – 1998:** PhD student at the Universities of Perugia and of Siena under the supervision of Prof. C. Petrongolo.

1995: CNR-fellowship at the ICQEM "Istituto di Chimica Quantistica ed Energetica Molecolare" of Pisa, under the supervision of Dr. A. Lami.

1992 – 1994: undergraduate student in the group of Theoretical Chemistry of the Department of Chemistry of Napoli under the supervision of Prof. G. Del Re.

International Research Experience

April 2003 – July 2003: Post Doc at the Physikalishes Institut, Universitaet Wuerzburg, Germany, in the research group of prof. G. Gerber, funded by the EU Network "COCOMO".

October 2000 – December 2000: Visiting Scholar at the Northwestern University, Evanston IL USA, in the research group of Prof. G. C. Schatz, funded by the CNR "Short-Mobility Program".

October 1993 – January 1994: "Free Mover Erasmus Student" at the Laboratory of Molecular Spectroscopy of the University "Claude Bernard" of Lyon, France, under the supervision of Prof. C. Barbier Chapelet, funded by the EU Erasmus Project.

Project Responsibility and Management

2016-2018 Principal Investigator of the ICCOM-CNR PROJECT: "SMODATA Model Development for Advanced Materials and Energy", DCM.AD002.261 involving 7 researchers

2013-2016 Principal Investigator of one Unit of the PRIN 2010-2011 Project 2010ERFKXL "Frontier studies in molecular spectroscopy and dynamics: from simple molecular systems to supramolecular aggregates and advanced materials"

2012-2015 Principal Investigator of the Italian node of the Project International Research Staff Exchange Scheme – Marie Curie Actions "Integrated Techniques in Structural Elucidation (InTechSE)"

2012-2015 Supervisor of a postdoctoral position funded by U-Mobility of University of Malaga (Spain) within Marie Curie Action, "Co-funding of Regional, National and International Programmes" for the project Theoretical study of Photoinduced processes and their spectroscopic marks. A quantum dynamical approach applied to DNA photophysics (T-T-PHANTASM)

2010-2013 Principal Investigator of the Pisa sub-unit of the IIT-SEED Project **"**Highly Efficient Modelling of Hybrid Organic Solar Cells (understanding the mechanism, improving the efficiency)". Project Leader dr. Filippo De Angelis ISTM-CNR

2010- Principal Investigator of the Research Unit of CNR "Models and methods for computational spectroscopy and the dynamics of charge- and energy-transfer phenomena"

2009 Principal Investigator of the Research Unit of CNR "Development and Application of multiscale models and methods for the study of nanosystems and nanostructures"

2006-2008 Principal Investigator of the Research Unit of CNR "Modelling of properties and reactivity of biological and bio-mimetic systems", MD.P01.013 involving 6.4 researchers per year**.**

Awards

2009: Award CNR "incentivazioni al personale anno 2005"

1996: Award Federchimica (the National Association of the Chemical Industries) "Toward an Intelligent Future", in a contest open to students graduated between 1993 and 1995 in Chemistry, Industrial Chemistry and Chemical Engineering.

Member of phD Committees

2014 September: Member of the Jury for the defense of the PhD thesis "Modelling of potential energy surfaces for photochemistry: Conical intersections and application to optical control" by Sergi Ruiz-Barrágan, at University of Gerona, Spain

2012 March: Member of the Jury for the defense of the PhD thesis "Ciclofanos quirais de 1,3-dietinilalenos: síntese, caracterización e estudo das súas propiedades quirópticas" by Inmaculada Rodríguez Lahoz at University of Vigo, Spain

2011 June: Opponent in the Jury for the defense of the PhD thesis "Theoretical studies of natural and magnetic circular dichroism, by Harald Solheim**"**, at University of Tromso, Norway

2011 May: Member of the Jury for the defense of the PhD thesis "Calculos quimico quanticos en sistemas hibridos formados por moleculas y nanoestructuras: procesos de transferencia de carga fotoinducida y reacciones quimicas" by Francisco Jose Avila Ferrer, University of Malaga, Spain

2011 June: Member of the Jury for the defense of the PhD thesis "Theoretical Studies on Photophysics and Photochemistry of DNA", by YuejieAi, KTH, Royal Institute of Technology, Stockholm, Sweden

2010 October Member of the Jury to award PhD positions in Chemical Science at University of Pisa

2010 Member of the Jury for the defense of the PhD thesis "Theoretical Studies on Kinetics of Molecular Excited States", by Feng Zhang, KTH, Royal Institute ot Technology, Stockholm, Sweden

Reviewer

JCR Journals

Fabrizio Santoro has been recently a reviewer for JACS, J Chem Phys, J Phys Chem, Chem Phys, Chem Phys Lett, Mol Phys, Chem Comm, Chem Sci, Spectr Chim Acta, PCCP, Chirality, J Mol Liq, J Mol Struct, J Chem Theor and Comp, Photoc. Photob. Sci., RSC Adv

Miscellaneous

Fabrizio Santoro has served as referee for German DFG for Post Doc applications for Belgian FNRS for Post Doc applications, for Italian ANVUR, and for Italian Minister MIUR for PRIN Projects.

Conference Organization

5) International workshop:
Dna-Day ELECTRONIC PROPERTIES OF DNA OLIGOMERS
A training ground for modelling and experiments

Pisa, 7 July 2016

4) WM12: Winter Modeling 2012,
Pisa 9 November, 2012

3) Primo Congresso della Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana,
Pisa 22-23 February, 2012

2) WM11: Winter Modeling 2011,
Pisa 13-14 January, 2011

1) WM08: Winter Modeling 2008,
Pisa 19 December, 2008

Research Interests Keywords

Photochemistry and photophysics; quantum and semi-classical dynamics; ultrafast dynamical processes in biological systems; nonadiabatic processes and dynamics at conical intersections; theory and computations of steady-state one-photon and two-photon spectroscopy in solution; theory and simulation of time-resolved spectroscopy; laser coherent control of molecular processes; excited states and dynamics of molecules embedded in a solvent; electron transfer in condensed phase.

Publications

120. J. Cerezo, A. Petrone, F. J. Avila Ferrer, G. Donati, F: Santoro, R. Improta, N. Rega
Electronic spectroscopy of a solvatochromic dye in water: comparison of static cluster/implicit and dynamical/explicit solvent models on structures and energies
Theor. Chem. Acc. accepted 2016

119. J. Cerezo, F. Santoro
Revisiting vertical models to simulate the line shape of electronic spectra adopting cartesian and internal coordinates
J. Chem. Theor. Comp. **DOI:**10.1021/acs.jctc.6b00442 2016

118. Y. Liu, J. Cerezo, F. Santoro, A. Rizzo, N. Lin, X. Zhao
Theoretical investigation of the broad one-photon absorption line-shape of a flexible symmetric carbazole derivative
Phys. Chem. Chem. Phys. **18**, 22889-22905, 2016

117 J. Cerezo, L. Fernandez Martinez, R. Improta, F. Santoro,
Vibronic approach to the calculation of decay rate of the photoexcited charge-transfer state of Guanine-Cytosine stacked dimer in water solution
Theor. Chem. Acc. **135**, 221, 2016

116 E. Stendardo, F. Avila Ferrer, F. Santoro, R. Improta
The absorption and emission spectra in solution of oligo-thiophene based push-pull biomarkers: a PCM/TD-DFT vibronic study
Theor. Chem. Acc. **135**, 150, 2016

115. Y. Liu, J. Cerezo, G. Mazzeo, N. Lin, X. Zhao, G. Longhi, S. Abbate, F. Santoro
Vibronic coupling explains the different shape of electronic circular dichroism and of circularly polarized luminescence spectra of hexahelicene
J. Chem. Theor. Comp. **12**, 2799-2819, 2016

114. J. Cerezo, F. Santoro, G. Prampolini
Comparing classical approaches with empirical or quantum-mechanically derived force fields for the simulation electronic lineshapes: application to coumarin dyes
Theor. Chem. Acc. **135**: 143(1-21), 2016

113. D. Padula, F. Santoro, G: Pescitelli
A Simple Dimeric Model Accounts for the Vibronic ECD Spectra of Chiral Polythiophenes in their Aggregated States
RSC Adv. **6**, 37938–37943, 2016

112 F. Santoro, D. Jacquemin
Going Beyond the Vertical Approximation with TD-DFT
Wiley Interdisciplinary Reviews: Computational Molecular Science, **6**, 460-487, 2016.
COVER IMAGE: Volume 6, Issue 5, 2016 DOI: 10.1002/wcms.1278

111. R. Improta, F. Santoro, L. Blancafort
Quantum Mechanical Studies on the Photophysics and the Photochemistry of Nucleic Acids and Nucleobases
Chem. Rev. **116**, 3540−3593, 2016

110. Irene Tosi, Mireia Segado Centellas, Elisa Campioli, Alessandro Iagatti, Andrea Lapini, Cristina Sissa, Laura Baldini, Chiara Cappelli, Mariangela Di Donato,Francesco Sansone, Fabrizio Santoro, Francesca Terenziani
Excitation dynamics in hetero-bichromophoric calixarene systems
ChemPhysChem **17**, 1 – 22, 2016

109. J. Cerezo, F. Avila Ferrer, G. Prampolini, F. Santoro
Modeling Solvent Broadening of the Vibronic Spectra of a Series of Coumarin Dyes. From Implicit to Explicit Solvent Models
J. Chem Theor and Comp **11**, 5810–5825, 2015

108. D. Padula, I. R. Lahoz, C. Díaz, F. E. Hernández, L. Di Bari, A. Rizzo, F. Santoro, M. M. Cid
A combined experimental-computational investigation to uncover the puzzling (chiro-)optical response of pyridocyclophanes: One- and two-photon spectra,
Chemistry Eur J. **21**, 12136-12147, 2015

107. F. Santoro
Quantum and Semiclassical Dynamics
In *Reference Modules in Chemistry, Molecular Science and Chemical Engineering*, In: Reedijk, J. (Ed.) Elsevier Reference
Module in Chemistry, Molecular Sciences and Chemical Engineering. Waltham, MA: Elsevier. 29-July-15 doi: 10.1016/B978-0-12-409547-2.10841-8.

106. J. Cerezo, F. Avila, F. Santoro

Disentangling vibronic and solvent broadening effects in the absorption spectra of coumarin derivatives for dyes sensitized solar cells
Phys Chem Chem Phys **17**, 11401-11411, 2015

105. A. Petrone, J. Cerezo, F. Avila, G. Donati, R. Improta, N. Rega, F. Santoro,
Absorption and emission spectra lineshape of a prototype dye in water by combining classical/dynamical and quantum/static approaches",
*J. Phys. Chem A.***119**, 5426–5438, 2015

104. T. Fahleson,J. Kauczor, P. Norman, F. Santoro, R.Improta, S. Coriani
TD-DFT investigation of the Magnetic Circular Dichroism Spectra of some purine and pyrimidine bases of nucleic acids
J. Phys. Chem. A **119**, 5476–5489, 2015

103. F. J. Avila Ferrer, M. D. Davari D. Morozov, G. Groenhof, F. Santoro
The lineshape of electronic spectra of GFP chromophore, part II: solution phase
Chem Phys Chem **15**, 3246-3257 2014

102. M. Di Donato, M. Segado Centellas, A.Lapini*, M. Lima, F. Avila, F. Santoro, C. Cappelli, R. Righini
A Combination of Transient 2D-IR Experiments and ab initio Computations Sheds Light on the Formation of the Charge-Transfer State in Photoexcited Carbonyl Carotenoids
J. Phys. Chem. B **118**, 9613-9630, 2014

101. M. D. Davari, F. J. Avila Ferrer, D. Morozov, F. Santoro, G. Groenhof
The lineshape of electronic spectra of GFP chromophore, part I: gas phase
Chem Phys Chem, **15**, 3236-3245 2014

100. R. Improta, F. J. Avila Ferrer, E. Stendardo, F. Santoro,
Quantum-classical calculation of the absorption and emission spectral shapes of oligothiophenes at low and room temperature by first-principle calculations,
Chem Phys Chem, **15**, 3320-3333, 2014

99. A. Chantzis, J. Cerezo, A. Perrier, F. Santoro, D. Jacquemin
Optical Properties of Diarylethenes with TD-DFT: 0-0 Energies, Fluorescence, Stokes Shifts and Vibronic Shapes
J. Chem Theor and Comp **10**, 3944-3957 (2014)

98. F. Santoro, R. Improta, T. Fahleson, J. Kauzcor, P.Norman, S. Coriani,
Relative Stability of the La and Lb Excited States in Adenine and Guanine: Direct Evidence from TD-DFT Calculations of MCD Spectra
J. Phys. Chem. Lett. 5, 1806−1811, 2014

97. F. Avila, J. Cerezo, J. Soto, R. Improta, F. Santoro
First-principle computation of absorption and fluorescence spectra in solution accounting for vibronic structure, temperature effects and solvent inhomogenous broadening
Comp. Theor. Chem **1040-1041**, 328-337, 2014

96. F. Avila, F. Santoro, R. Improta
The excited state behavior of cytosine in the gas phase: A TD-DFT study
Comp. Theor. Chem **1040-1041**, 186-194, 2014

95. A Lapini, P Fabbrizzi, M. Piccardo, M.di Donato, L. Lascialfari, P. Foggi, S. Cicchi, M.Biczysko, I. Carnimeo, F. Santoro, C..Cappelli, R. Righini
Ultrafast resonance energy transfer in the umbelliferone–alizarin bichromophore,
PCCP **16**, 10059-10074, 2014

94. P. Scafato, F. Caprioli, L. Pisani, D. Padula, F. Santoro, G. Mazzeo, S. Abbate, F. Lebon, G. Longhi
Combined use of three forms of chiroptical spectroscopies in the study of the absolute configuration and conformational properties of 3-phenylcyclopentanone, 3-phenyl cyclohexanone,
Tetrahedron **69**, 10752-10762, 2013

93. J. Cerezo, J. Zuniga, A. Requena, F. Avila Ferrer, F. Santoro
Harmonic models in Cartesian and internal coordinates to simulate the absorption spectra of carotenoids at finite temperatures;
J. Chem. Theor. Comp. **9**, 4947-4958, 2013. Erratum: *J. Chem. Theory Comput.*, **2014**,*10*, 3586–3587

92. G. Pescitelli, V. Barone, L. Di Bari, A. Rizzo, F. Santoro
Vibronic Coupling Dominates the Electronic Circular Dichroism of the Benzene Chromophore ^1L_b band
J. Org. Chem. **78**, 7398-7405, 2013 (selected as featured article)

91. F. Avila , V. Barone, C. Cappelli, F. Santoro
Duschinsky, Herzberg-Teller and multiple electronic resonance interferential effects in resonance Raman spectra and excitation profiles. The case of pyrene
J. Chem. Theor. Comp. **9**, 3597-3611, 2013

90. F. Santoro, R. Improta, F. Avila, M. Segado, A. Lami,
The interplay between neutral exciton and charge transfer states in single-strand polyadenine. A quantum dynamical investigation
Photoc. Photob. Sci. **12**, 1527-1543 (2013)

89. N. Lin, V. Barone, C. Cappelli, X. Zhao, K. Ruud, F. Santoro
Effective time-independent studies on resonance Raman spectroscopy of trans-stilbene including Duschinsky effect
Mol. Phys. **111**, 1511-1525, (2013)

88. D. Padula, D. Picconi, A. Lami, A. Lami, F. Santoro
Electronic Circular Dichroism in Exciton-Coupled Dimers: Vibronic Spectra from a General All-Coordinates Quantum-Dynamical Approach
J. Phys. Chem. A **117**, 3355–3368 (2013)

87. N. Lin, H. Solheim, X. Zhao, F. Santoro, K. Ruud
First Principles Studies on the Vibrationally Resolved Magnetic Circular Dichroism Spectra of Biphenylene
J. Chem. Theor. Comp. **9**, 1557-1567 (2013)

86. D. Picconi, F. Avila, A. Lami, R. Improta, F. Santoro

Quantum-classical effective-modes dynamics of the pp* ! np* decay in 9H-adenine. A quadratic vibronic coupling model
Faraday Discuss. **163**, 223-242, (2013)

85. F. Avila, J. Cerezo, E. Stendardo, R, Improta, F. Santoro
Insights for an Accurate Comparison of Computational Data to Experimental Absorption and Emission Spectra: Beyond the Vertical Transition Approximation
J. Chem . Theor. Comp. **9**, 2072-2082 (2013)

84. G. Pescitelli, D. Padula, F. Santoro
Intermolecular Exciton Coupling and Vibronic Effects in Solid-State Circular Dichroism: A Case Study
Phys. Chem. Chem. Phys. **15**, 795-802, (2013)

83. E. Stendardo, F. Avila, F. Santoro, R. Improta,
Vibrationally Resolved Absorption and Emission Spectra of Dithiophene in the Gas Phase and in Solution by First-Principle Quantum Mechanical Calculations
J. Chem.. Theor. Comp. **8**, 4483-4493, (2012)

82. A. Weigel, M. Pfaffe, M. Sajadi, R. Mahrwald, R. Improta, V. Barone, D. Polli, G. Cerullo, N. P Ernsting, F. Santoro
Barrierless photoisomerisation of the "simplest cyanine": Joining computational and femtosecond optical spectroscopies to trace the full reaction path
Phys Chem Chem Phys **14**, 13350-13364, (2012)

81. D. Padula, L. Di Bari, F. Santoro, H. Gerlach, A. Rizzo
Analysis of the Electronic Circular Dichroism Spectrum of (-)–[9](2,5)Pyridinophane
Chirality **24**, 994-1004 (2012)

80. F. Avila, F. Santoro
Comparison of Vertical and Adiabatic Harmonic Approaches for the Calculation of the Vibrational Structure of Electronic Spectra
Phys Chem Chem Phys **14**, 13549-13563 (2012)

79. D. Picconi, A. Lami, F.Santoro
Hierarchical transformation of Hamiltonians with linear and quadratic couplings for nonadiabatic quantum dynamics: Application to the ππ*/nπ* internal conversion in thymine
J Chem Phys **136**, 244104-1/17 (2012)

78. M. Biczysko, J. Bloino, G. Brancato, I. Cacelli, C. Cappelli, A. Ferretti, A. Lami, S. Monti, A. Pedone, G. Prampolini, C. Puzzarini, F. Santoro, F. Trani, G. Villani
Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case
Theor. Chem. Acc. **131**, 1201-1/19 (2012)

77. N. Lin, H. Solheim, K. Ruud, M. Nooijen, F. Santoro, X. Zhao, M. Kwit, P. Skowroneke
Vibrationally resolved circular dichroism spectra of a molecule with isotopically engendered chirality
Phys Chem Chem Phys **14**, 3669-3680 (2012)

76. F. J. Avila Ferrer, R. Improta, F. Santoro, V. Barone
Computing the inhomogeneous broadening of electronic transitions in solution: a first-principle quantum mechanical approach
Phys Chem Chem Phys **13**, 17007-17012 (2011)

75. N. Lin, Y. Luo, X. Zhao, K. Ruud, F. Santoro, A. Rizzo
Difference in Two-photon and One-photon Absorption Profiles Induced by Vibronic Coupling: The Case of Dioxaborine Heterocyclic Dye
Chem Phys Chem. **12**, 3392-3403 (2011)

74. D. Picconi, V.Barone, A. Lami, F. Santoro, R.Improta
The interplay between pipi* and npi* lowest excited states in nonradiative decay of photoexcited thymine
Chem Phys Chem **12**, 1957-1968 (2011)

73. F. Santoro, C. Cappelli, V. Barone,
Efficient time-independent method for the calculation of resonance Raman spectra in sizeable molecules including Duschinsky and Herzberg-Teller effects
J. Comp. Theory and Comp **7**, 1824-1839 (2011).

72. N. Lin, F. Santoro, X. Zhao, C. Toro, L. De Boni, F. E. Hernandez, A. Rizzo
Computational challenges in simulating and analyzing experimental linear and nonlinear circular dichroism spectra. R-(+)-1,1'-bi(2-naphtol) as a prototype case.
J. Phys Chem B **115**, 811-824 (2011)

71. A. Lami, F. Santoro,
Time-dependent approaches to the calculation of steady-state vibronic spectra. From fully quantum to classical approaches,
in Computational Strategies for Spectroscopy: from Small Molecules to Nano Systems*, ed. V. Barone, Wiley, Chichester, UK, 2011, pp.* 475-516. ISBN: 978-0-470-47017-6

70. M. Biczysko, J. Bloino, F. Santoro, V. Barone
Time-independent approaches to simulate electronic spectra lineshapes. From small molecules to macrosystems
in Computational Strategies for Spectroscopy: from Small Molecules to Nano Systems*, ed. V. Barone, Wiley, Chichester, UK, 2011, pp.* 361-446. ISBN: 978-0-470-47017-6

69. P. Rivera-Fuentes, J.L. Alonso-Gómez, A. G. Petrovic, F. Santoro, N. Harada, N. Berova, F. Diederich
Optically Enantiomerically Pure Alleno-acetylenic Macrocycles: Synthesis, Solid State Structures, Chiroptical Properties, and Electron Localization Function Analysis
Chemistry -A European Journal **16,** 9786-9797 (2010)

68. C. Toro, L. De Boni, N. Lin, F. Santoro, A. Rizzo, and F. E. Hernandez
Two-photon circular-linear dichroism on axial enantiomers,
Chirality, **22** E202-E210 (2010)

67. F. Santoro, V. Barone, A. Lami, R. Improta
The excited states of adenine-guanine stacked dimers in aqueous solution: a PCM/TD-DFT study

Phys. Chem. Chem. Phys. **12,** 4934-4948 (2010)

66. J. Bloino, M. Biczysko, F. Santoro, V. Barone
General approach to compute vibrationally resolved one-photon electronic spectra
J. Comp. Theory and Comp. **6**, 1256-1274 (2010).

65. C. Toro, L. De Boni, N. Lin, F. Santoro, A. Rizzo, and F. E. Hernandez
Two-photon absorption circular dichroism: A new twist in nonlinear spectroscopy
Chemistry- A European Journal **16,** 3504-3509 (2010)

64. P. Rivera-Fuentes, J.L. Alonso-Gómez, A. G. Petrovic, F. Santoro, N. Harada, N. Berova, F. Diederich,
Amplification of Chirality in Monodisperse, Enantiopure Alleno-Acetylenic Oligomers
Angew. Chem. Int. Ed., **49,** 2247-2250, (2010).

63. F. Santoro, V. Barone
Computational approach to the study of the lineshape of absorption and electronic circular dichroism spectra
Int. J. Quantum. Chem **110**, 624-636, (2010)

62. R. Improta, A. Lami, V. Barone, F. Santoro
Time-dependent and time-independent approaches for the computation of absorption spectra of Uracil derivatives in solution.
Int. J. Quantum .Chem. **110**, 476-486, (2010)

61. R. Improta, F. Santoro, V. Barone, A. Lami,
Vibronic Model for the quantum dynamical study of the competition between bright and charge-transfer excited states in single-strand polynucleotides: the adenine dimer case
J. Phys. Chem. A **113**, 15346-15354 (2009)

60. R. Improta, V. Barone, A. Lami, F. Santoro
Quantum Dynamics of the ultrafast ππ*/nπ population transfer in Uracil and 5Fluoro-Uracil in water and acetonitrile.
J. Phys. Chem B **113**, 14491-14503, (2009)

59. F. Santoro, V. Barone, R. Improta
The excited states decay of the A-T DNA: a PCM/TD-DFT study in aqueous solution of the (9-methyl-adenine)$_2$(1-methyl-thymine)$_2$ stacked tetramer
J. Am. Chem. Soc. **131**, 15232-15245, (2009).

58. C. Angeli, R. Improta, F. Santoro
On the controversial nature of the 1^1Bu and 2^1Bu states of trans-stilbene: the n-electron valence state perturbation theory approach
J. Chem. Phys **130**, 174307/1-6 (2009)

57. F.Santoro, R. Improta, V. Barone
Three-Dimensional Diabatic Models for the $\pi\pi^* \rightarrow n\pi^*$ Excited-State Decay of Uracil Derivatives in Solution
Theor. Chem. Accounts, **123**, 273-286 (2009)

56. N. Lin, F. Santoro, A. Rizzo, Y. Luo, X. Zhao, , V. Barone

Theory for vibrationally resolved two-photon circular dichroism spectra. Application to (R)-(+)-3-methylcyclopentanone
J Phys. Chem A. **113**, 4198-4207 (2009)

55. V. Barone, J. Bloino, M. Biczysko, F. Santoro
Fully integrated approach to compute vibrationally resolved optical spectra: from small molecules to macrosystems
J. Comp. Theory and Comp. **5**, 540-554 (2009)

54. L. Barsanti, P. Coltelli, V. Evangelista, V. Passarelli, A. M. Frassanito, N. Vesentini, F. Santoro, P. Gualtieri
In vivo absorption spectra of the two stable states of the *Euglena* photoreceptor photocycle
Photochem. and Photobiol. **85**, 304-312 (2009)

53. F. Santoro, V. Barone, R. Improta
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Talks and Posters at Conferences and Meetings

58. **F. Santoro**
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Bordeaux, Febbraio 2016

56. **F. Santoro**
Frontier studies in molecular spectroscopy and dynamics: from simple molecular systems to supramolecular aggregates and advanced materials. The activity of Pisa Unit
Final meeting of PRIN Project 2010-20**11**
Bologna, Febbraio 2016

55. **F. Santoro**
ThC^2-Lab: Modeling for Advanced Materials
Giornate Scientifiche del Dipartimento di Scienze Chimiche e Tecnologie dei Materiali
Cetraro, Ottobre 2015

54. **F. Santoro,**
Vibronic Approaches to the Calculation of Optical Chiral Spectra
II Workshop ChirItaly,
Rome September 2015

53. **F. Santoro,**
Vibronic Approaches to the Calculation of Optical Chiral Spectra
Chirality 2015,
Boston, July 2015

52. **F.Santoro**,

Quantum/Classical Dynamical Approaches for the Calculation of Vibronic Chiral Spectra, Final Marie-Curie InTechSe Workshop
Vigo, June 2015

51. **F.Santoro,**
Toward the simulation of optical and chiroptical properties of polythiophenes. Hybrid quantum/classical dynamical approaches,
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Bangalore, March 2015

50. **F. Santoro**,
Recent progresses towards the time-dependent calculation of vibronic spectra of flexible and (or) nonadiabatic systems
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Houffalize, Sep 2014

49. **F. Santoro**,
Time dependent approaches for vibronic spectra and internal conversion rates in large systems
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48. **F. Santoro**,
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47. **F. Santoro,**
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45 **F. Santoro,**
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44. **F. Santoro,**
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43. **F. Santoro,**
Investigation and simulation of chiroptical properties: The expertise of Pisa Unit
Meeting of the Marie Curie INtechSe Project
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42. **F. Santoro**,
Electronic Circular Dichroism in excitonic-coupled dimers: A general all-coordinates quantum-dynamical approach
Molecules at the Mirror -- Chirality in Chemistry and Biophysics, Molecole allo Specchio: Chiralità in Chimica e Biofisica,
Roma, Oct 2012 (contributed talk)

41. D. Padula, D. Picconi, A. Lami, G. Pescitelli, L. Di Bari, **F. Santoro**
Quantum dynamical approach for the calculation of vibrationally resolved ECD spectra induced by exciton couplings
CECAM Workshop Vibrational Optical Activity: Interplay of Theory and Experiment
Pisa, Sept 2012 (poster)

40. F. Avila, V. Barone, C. Cappelli, A. Lami, D. Picconi, **F. Santoro**
Vibronic effects in basic molecular aspects of solar energy conversion: light harvesting, charge and energy transfer
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Chia Laguna, Sept 2012 (poster)

39. A. Avila, **F. Santoro**,
Comparison of vertical and adiabatic harmonic approaches for the Calculation of the vibrational structure of electronic spectra
Primo Congresso Nazionale della Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana
Pisa, Feb 2012 (poster)

38. **F. Santoro**,
Monomeric and collective deactivation mechanisms in photoexcited DNA investigated by a quantum dynamical approach
XXIV Congresso Nazionale della SCI,
Lecce, Sept 2011 (contributed talk)

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Lausanne (CH), Nov 2010 (invited talk)

36. **F. Santoro**,
Quantum Computational approaches to biochemical processes
XVI Scuola Nazionale di Scienza dei Materiali
Bressanone, Sept 2010 (invited lecture)

35. **F. Santoro**,
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Stresa, Sept 2010 (invited keynote lecture)

34. **F. Santoro**,
Vibrational Strucutre of one- and two-photon electronic spectra of large semirigid molecules
International Workshop "Polar 2010",
Tromso (NO), June 2010, (invited talk)

33. **F. Santoro**,
Nonadiabatic decay of photoexcited DNA. A quantum dynamical study of single nucleobases and oligomers
International Meeting "Multiscale Modeling in Simulation and Science,
Stockholm, Nov 2009 (invited talk)

32. **F. Santoro**,
A hierarchy of models to describe vibrational effects in optical spectra of large molecules
International Meeting "Multiscale Modeling in Simulation and Science,
Stockholm, Nov 2009 (invited lecture)

31. **F. Santoro**,
Time-dependent and time-independent approaches to the computation of vibrationally resolved electronic spectra
5th International Meeting "Mathematical Methods for Ab initio Quantum Chemistry",
Nice , Oct 2009. (Invited lecture)

30. **F. Santoro**, V. Barone, A. Lami, R. Improta
Quantum dynamics of the photodeactivation mechanisms in DNA single nucleobases and oligomers
24th International Conference on Photochemistry,
Toledo (Spain), Jul 2009 (contributed talk)

29. **F. Santoro**,
A time-independent approach to the computation of vibrationally-resolved electronic spectra
XIV European Seminar on Computational Methods in Quantum Chemistry
Isola d'Elba, Oct 2008 (invited talk)

28. **F. Santoro**
A 3D Model for Isomerization of a molecular switch mimicking retinal.
Meeting "Development of ultrafast light driven molecular motors"
Zurich, Sept 2008 (invited talk)

27. **F. Santoro**,
Quantum dynamics of ultrafast photoinduced processes in biological molecules. The cases of Uracil and Retinal
ChiTel08, XXXIV Congresso dei Chimici Teorici di Espressione Latina,
Cetraro, Jul 2008 (invited plenary)

26. **F. Santoro**,
Computational Vibrationally-Resolved Optical Spectra,
European Workshop CERC3,
Perugia May 2008 (invited talk)

25. **F. Santoro**,
I progetti di Modeling nel Dipartimento Materiali e Dispositivi,
Workshop "Winter Modeling 2007-Modeling per i Materiali Nanostrutturati, i Biosistemi e l'Ambiente",
Roma, Nov 2007 (invited talk)

24. **F.Santoro**, V. Barone, R. Improta, A. Lami,, M. Olivucci,
Quantum dynamics of ultrafast photoinduced processes in biological molecules,
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Conference Femtochemistry and Femtobiology 8,
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21. **F. Santoro**, R. Improta
Dynamics of the photodeactivation process in DNA nucleobases,
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Gallipoli (LE), Jun 2007. (talk)

20. **F. Santoro**, R. Improta, A. Lami, J. Bloino, V. Barone,
An effective method to compute vibrationally resolved optical spectra of large molecules in solution including Duschinsky, temperature and Herzberg-Teller effects,
Workshop Progress in ab initio modelling of biomolecules : towards computational spectroscopy,
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19. **F.Santoro**, A.Lami, R. Improta, V. Barone
Un metodo efficiente per il calcolo di spettri di assorbimento di molecole di grandi dimensioni in soluzione,
Congresso GICC06,
Venezia S. Servolo, Dec 2006. (talk)

18. **F.Santoro**
Modellizzazione di proprietà e reattività di molecole biologiche e biomimetiche,
Meeting dei responsabili di Commessa del Progetto "Soft Matter", del Dipartimento Materiali e Dispositivi del CNR,
Roma, Oct 2006. (invited talk)

17. A. Ferretti, **F. Santoro**
Computational study of the chemisorption of sylil readicals on the Pd(100) surface.
MMD Meeting, Matter Materials and Devices,
Genova, Jun 2005. (poster)

16. A. Lami, M. Olivucci, **F. Santoro**
A tiny barrier can induce a bi-exponential decay of the retinal chromofore. A quantum dynamics investigation,
MMD Meeting, Matter Materials and Devices",
Genova, Jun 2005. (poster)

15. R. Improta**, F. Santoro**
The excited state behavior of stilbene and stiff-stilbene. A TD-DFT study
XXXIV Congresso Nazionale di Chimica Fisica,
Siena, Jun 2005. (poster)

14. **F. Santoro**, R. Improta, P. Nuernberger, G. Vogt, G. Gerber
A comparative experimental and theoretical study of the photoisomerization of thiacyanine
VII Conference "Complex Systems: structure, properties, reactivity and dynamics.", Alghero, Jun 2005. (talk)

13. A. Lami, M. Olivucci, **F. Santoro**
The photoisomerization of retinal. Effects of the plateau on the S_1 reactive surface: a quantum and classical dynamical study
CCP6 Workshop "Quantum Dynamics at Conical Intersections",
Nunspeet (Netherlands), Sept 2004. (poster)

12. R. Improta**, F. Santoro**,
A theoretical investigation on the factors influencing cyanine photoisomerization: the case of thiacyanine in gas phase and in methanol
XXXIII Congresso Nazionale di Chimica Fisica,
Napoli, Jun 2004. (poster)

11. A. Lami, M. Olivucci, **F. Santoro**
The photoisomerization of retinal. Effects of the plateau on the S_1 reactive surface: a quantum and classical dynamical study,
XXXIII Congresso Nazionale di Chimica Fisica,
Napoli, Jun 2004. (talk)

10. A. Lami, **F. Santoro**
Robust laser control by a weak multicolor laser pulse of the fluorescence of NO2 from the X^2A'/A^2A' conical intersection,
Summer School in Coherent Control in Atomic and Molecular Systems,
Cargese (France), Oct 2002 (talk)

9. A. Lami, **F. Santoro**
Laser control in multilevel systems by a weak-intensity multicolor gaussian pulse
Vth Femtochemistry Conference,
Toledo (Spain), Sept 2001 (poster)

8. **F.Santoro,** C. Petrongolo and G. C. Schatz,
Effetti Renner Teller nella dinamica della reazione $N(^2D) + H_2\ (X\,^1\Sigma_g^+) = NH\ (X\,^3\Sigma^- + a\,^1\Delta) + H\ (^2S)$,
XXXI Congresso Nazionale di Chimica Fisica,
Padova, Jun 2001. (talk)

7. **F.Santoro,** C. Petrongolo and G. C. Schatz,
Effetti Renner Teller nella reazione $N(^2D) + H_2\ (X\,^1\Sigma_g^+) = NH\ (X\,^3\Sigma^- + a\,^1\Delta) + H\ (^2S)$
Scientific Meeting of the Research Project (coordinator Prof. Gianturco) funded by MURST,
Pisa, Feb 2001. (talk)

6. **F. Santoro**, C. Petrongolo and A. Lami,
Time- and frequency- resolved nonadiabatic spontaneous emission of NO_2,
International Conference "Atoms Molecules and Quantum Dots in Laser Fields",
Pisa Jun 2000. (poster)

5. **F. Santoro**, C. Petrongolo
Spettri di fluorescenza di NO_2 *risolti nel dominio del tempo e della frequenza*,
Congresso dei Chimici Teorici di Espressione Latina, ChiTel99,
Napoli, Sept 1999. (poster)

4. **F. Santoro**, C. Petrongolo
$\tilde{X}\,^2A_1/\tilde{A}\,^2B_2$ *conical intersection effects on the radiative lifetimes and fluorescence spectra of* NO_2
IV Convegno Sistemi Complessi: Struttura, proprietà, reattività e dinamica,
Varenna, Jun 1999. (talk)

3. **F. Santoro**, C. Petrongolo,
$\tilde{X}\,^2A_1/\tilde{A}\,^2B_2$ *conical intersection effects on the absorption spectrum and the wavepacket dynamics of* NO_2
European Conference on Atomic and Molecular Physics,
Siena, Jul 1998. (poster)

2. R. Brandi, **F. Santoro**
L'intersezione conica $\tilde{X}\,^2A_1/\tilde{A}\,^2B_2$ *di* NO_2*: calcolo dello spettro di assorbimento non adiabatico in approssimazione di Franck-Condon,*
Seminario Nazionale di Chimica Fisica, Fotochimica,
Torino, Jun 1997. (poster)

1. A. Lami, **F. Santoro**
Effetti dissipativi sul trasferimento elettronico intramolecolare.
Conference "Verso la complessità molecolare: modelli per la dinamica ed i processi reattivi",
Monselice, June 1995. (talk)

N.B.. Only contributions presented by F. Santoro are listed. F. Santoro also co-authored dozens of posters and talks presented by other authors

Invited Seminars

15. **F. Santoro**
Calculation of Steady-State Vibronic Spectra: From fully Quantum to hybrid Quantum/ Classical Approaches
Goethe Universitaet, Frankfurt November 19, 2015

14. **F. Santoro**
Computational electronic spectroscopy: From the vertical transition approach to the simulation of line shapes
Virginia Tech, Blacksburg VA, July 3rd 2015

13. **F. Santoro**
Quantum/Classical Dynamical Approaches for the Calculation of Vibronic Spectra in Complex Systems
Gaussian Inc. Wallingford CN, June 25 2015

12. **F. Santoro,**
Time-dependent calculation of vibronic spectra. Possible strategies for flexible and (or) nonadiabatic systems
Chemistry Department, University of Parma, 12 Feb 2015

11. **F. Santoro,**
Recent progresses towards the time-dependent calculation of vibronic spectra of flexible and (or) nonadiabatic systems
Chemistry Department, University of Düsseldorf, 14 Jan 2015

10. **F. Santoro**
Recent progresses towards the time-dependent calculation of vibronic spectra of flexible and (or) nonadiabatic systems
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Code Development

Fabrizio Santoro is the developer of number of codes for computational chemistry applications. Among the others is the author of a suite of Fortran codes for the computation of the vibrational structure of several kinds of electronic spectra, namely absorption, emission, circular dichroism, two-photon absorption, two-photon circular dichroism, resonance Raman. A standard version of the code can be freely downloaded at http://www.pi.iccom.cnr.it/fcclasses. At present, the code has been downloaded more than 200 times and adopted in dozens of scientific publications