Raffaele Borrelli

Personal Data

First name:	Raffaele
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Born:	April, 17th 1976 in Napoli (Italy)
Nationality:	Italian
Languages:	Italian (mother language), English (fluent), German (Intermediate)
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Current Position

Associate Professor – University of Torino.

Education

1999, Nov - 2003, Mar Ph. D. in Chemistry, University of Salerno. *Ph. D. Thesis:* "Quantum Dynamics of Ultrafast Chemical Processes", advisor Prof. A. Peluso.

1994, Sep - 1999, Oct Degree in Chemistry, University of Napoli "Federico II". *Thesis:* "Theoretical Study of Electron Transfer Process in the Mechanism of Aromatic Nitration"; advisor Prof. G. Del Re. *Final mark:* 110/110 *cum laude*.

Research and Professional Experience

2011, Nov - 2019, Oct Assistant Professor position, Department of Agricultural Forestry and Food Science, University of Torino, Torino (Italy).

2019, March 2-March 18 Guest researcher at the University of Kyoto, Japan. Research group of Prof. Yoshitaka Tanimura.

2015, April 15-May 02 Guest researcher at School of Material Science and Engineering, Nanyang Technological University, Singapore. Research group of Prof. Yang Zhao. Research topic "Energy transfer dynamics in photosynthesis and femtosecond spectroscopy".

2015, March-April Guest researcher at Chemistry Department of the Technische Universität München. Research group of Prof. Wolfgang Domcke. Research topic "Photocathalytic Water-splitting Systems".

2014, June Guest researcher at Chemistry Department of the Technische Universität München, in the research group of Prof. Wolfgang Domcke. Research topic "Photocathalytic Water-splitting Systems".

2009, Oct - 2010, Oct Guest researcher at Chemistry Department of the Technische Universität München, in the research group of Prof. W. Domcke. Research topic "Water splitting in Magnesium-porphyrin-Quinone Systems".

2009, May - 2009, June Guest researcher at Chemistry Department of the Technische Universität München, in the research group of Prof. W. Domcke. Research topic "Dynamics and Intermediates of Molecular Transformations".

2006, Mar-2011, Nov Assistant Professor position, Department of Chemistry, University of Salerno, Salerno (Italy).

2005, Jul - 2006, Mar Post-Doc position, Department of Chemistry of the University of Salerno, Salerno (Italy). Research topic "Electron Transfer in Photosynthesis".

2004, Apr - 2005, May Researcher at the Italian Aerospace Research Center (C.I.R.A. Scpa). Activity field "Ceramic Materials for Ultra High Temperature Applications".

2003, Apr - 2004, Apr Post-Doc position, Department of Chemistry of the University of Salerno, Salerno (Italy). Research topic "Quantum Dynamics of Complex Systems".

2001, Nov - 2002, Aug Visiting graduate student at the Laboratories for Molecular Sciences, under the supervision of Prof. Ahmed H. Zewail, California Institute of Technology, Pasadena, California (USA). Research topic "Photophysics of Zinc-Porphyrin systems".

Fellowships

- Japan Society for the Promotion of Science (JSPS) Invitational Fellowships for Research in Japan FY2021, 1/4/2022 - 3/7/2022, topic "Modeling and analyzing proton-coupled electron transfer processes for solar energy production".
- Short term research fellowship, School of Materials Science and Engineering, Nanyang Technological University, Prof. Yang Zhao, 20/4/2015 - 1/5/2015, topic "Energy transfer dynamics in photosynthesis and femtosecond spectroscopy".
- DAAD Research Fellowship, Technische Universität München, Garching, topic "Photoinitiated proton coupled electron transfer", March 2015.
- DFG Research Fellowship, Technische Universität München, Prof. W. Domcke, "Excited-state dynamics of DNA base pairs" Garching, Germany, 1/10/2009 - 1/10/2010.

Presentations

- **Conferences Talks**

  ***2021*:** "Non-Equilibrium Thermo Field Dynamics and Tensor-Train Approaches to Closed and Open System Evolution: Theory, Implementation and Application", on-line workshop VISTA, Virtual International Seminar on Theoretical Advancements, 16/9/021.

  ***2021*:** "Tensor-trains methodologies in electron-vibrational problems: Closed and open systems theories", invited speaker atthe "The International Chemical Congress of Pacific Basin Societies 2021" (Pacifichem 2021), Dec 16-21 2021, Honululu, Hawaii, USA (on-line).

  ***2018*:** *Quantum Dynamics of Complex Molecular Systems at Finite Temperature: Thermo Field Dynamics approach*, High Dimensional Quantum Dynamics 2018 August 28-31, 2018, Lille, France.

  ***2018*:** *Dynamics and Spectroscopy of Complex Molecular Systems at Finite Temperature*, QueBS 2018 July 10-13, 2018, Vilnius, Lituania.

  ***2017*:** *Quantum Dynamics and Spectroscopy of Complex Molecular Systems at Finite Temperature*, Spectroscopy and Dynamics of Molecules and Clusters (SDMC2017), February 16-19, 2017, Pondicherry, India.

  ***2016*:** *Generalized Coherent States in Electronic Transitions: Methodology and Applications*, Summit Meeting 2016, September 23, 2016 - The National Academy of Sciences of Belarus, B. I. Stepanov Institute of Physics.

  ***2015*:** *Polaron time propagation in bridged molecular systems* Numerical Modeling in Evolutionary Problems: Perspectives and Applications, October 26-27, 2015, University of Salerno, Salerno, Italy.

  ***2015*:** *Quantum dynamics and kinetics of electron transfer in systems of biochemical interest*, Third Workshop on Coherent Energy Transport and Optimization in Photosynthesis, CETOP 2015, May 1-3, 2015, Nanyang Technological University, Singapore.

  ***2010*:** *Development of theoretical models of photocatalytic water splitting*, Munich-Center for Advanced Photonics, 2010, München, Germany.

  ***2006*:** *Franck-Condon Integrals Calculation and their use in the Study of Electronic States Transitions*, "XXXV Congresso di Chimica Fisica", September 10-15, 2006, Firenze (Italy).

- **Invited Seminars**

  ***2021*:** University of Kyoto. "The Energy Quest in Modern Physical Chemistry: a theoretical perspective", Feb 21 - Feb 24, 2022.

  ***2019*:** University of Kyoto. "From quantum dynamics to rate theories in complex molecular systems: analysis of electron transfer processes", March 4 and March 5, 2019.

  ***2019*:** Technical University of Munich (TUM). "Electron and energy transfer in biochemical and artificial systems: analogies and differences from a theoretical perspective", January 14, 2019.

  ***2017*:** Southern University of Science and Technology of China (SUSTC). "Thermal Fields in Dynamics and Spectroscopy of Complex Molecular Systems", March 2, 2017.

  ***2016*:** Technische Universität München, "Quantum electron-vibrational dynamics in molecular aggregates: methodologies and applications ", September 26, 2016.

  ***2016*:** Laboratoire de Chimie-Physique, Université Paris Sud, Orsay, "Quantum dynamics and kinetics of electron-transfer in systems of biochemical interest", May 30, 2016.

  ***2010*:** Max Planck Institute for the Physics of Complex Systems, Dresden "Quantum dynamics of electron-transfer in early ET steps of photosynthesi", April 1, 2010

  ***2009*:** Technische Universität München, "Quantum Dynamics of the early Electron Transfer steps in Bacterial Photosynthesis", May 28, 2009.

- **Posters and Papers at Congresses**

  ***2010*:** *Mechanistic aspects of photocatalytic water splitting: a vibronic model of the photoinduced electron transfer between porphyrin and quinone*, Bunsen Discussion Meeting on Light Harvesting and Solar Energy Conversion, March 28-30 2010, Stüttgart (Germany).

  ***2007*:** *Franck-Condon Analysis of the electron photodetachment spectrum of SF_6^- : a comparison of DFT and MP2 results*, DFT2007, 26-30 August 2007, Amsterdam, (The Netherlands).

  ***2004*:** *Advanced Ceramic Materials and related Technologies for Slender Shaped Hot Structure*, "55-th International Astronautical Congress", 4-8 October 2004, Vancouver (Canada).

  ***2001*:** *Theoretical and Spectroscopic study of non-radiative decay in Hemiporphyrazine*, "STC2001, 37-th Symposium for Theoretical Chemistry", 23-27 September 2001, Bad-Herrenalb (Germany).

  ***2001*:** *Electron Transfer in Aromatic Nitration*, "Tulip Graduate School, Modern Developments in Spectroscopy", 1-4 May 2001, Nordwjk, (The Netherlands).

Research Activity

- **Quantum Molecular Dynamics**

  My research activity in this field has been mainly devoted to the development and implementation of theoretical methodologies for the study of quantum dynamics in complex molecular systems.

  Starting from my early career, I have developed several methods for the time propagation of molecular wavepackets. I have implemented new techniques for the construction of vibronic Hamiltonians using Franck-Condon integrals, and employed Lanczos or Chebyshev methods for the numerical solution of the Schrödinger equation.

  A large effort of my research has been concentrated on the challenging problem of simulating the quantum dynamics of systems with many nuclear degrees of freedom. In this respect, I have developed *i*) new *pruning* techniques of the Hilbert space specifically tailored to handle electron transfer processes, *ii*) a simplified Markovian approach for the study of electronic transition based on cumulant theory, *iii*) a methodology to describe polaron and exciton dynamics based on the use of Generalized Coherent States.

  A significant breakthrough achieved in my research has been the development of a new methodology for quantum dynamical simulations at finite temperature using Thermo Field Dynamics theory combined with Tensor-Train numerical techniques (Borrelli, Gelin *J. Chem. Phys.* 2016). The method is able to describe exact quantum electron-vibration dynamics, including temperature effects, for systems with hundreds degrees of freedom.

- **Molecular Spectroscopy**

  My main achievement in this field has been the development of methodologies for the simulation of electronic spectra based either on the direct calculation of Franck-Condon integrals, or on the time-dependent approach obtained from Kubo-Toyozawa-Lax theory. Both methods allow to take into account Duschinsky and Herberg-Teller effects. This project started as part of my Post-doctoral position at the University of Salerno and is still ongoing.

  Furthermore, in collaboration with Prof. A. Peluso, new methodologies have been developed which include the use of curvilinear coordinates. Their implementation has allowed to shed light on some controversial electronic spectra such as those of NH_3, SF_6^-, $C_4F_8^-$, porphyrins, and organic dyes for applications in dye-sensitised solar cells.

  The methodologies have been implemented in the MolFC software, which is interfaced with several electronic structure calculation packages, such as Gaussian, Molpro, Turbomole and Gamess. The software is currently used by a large number of research groups, in the international scientific community, for the study of a variety of electronic and photoelectronic spectroscopy problems. This is confirmed by the significative number of scientific publications in which MolFC has been used.

  The software is freely distributed on the web site
  `http://github.com/rborrelli/molfc`.

- **Electron Transfer Theory**

  Since my early studies I have been working on the development of theoretical models to describe vibronically induced electron-trasfer reactions in chemical systems.

I have worked on a systematic theoretical study of the quantum dynamics of the electron transfer (ET) processes which take place between the cofactors of natural photosynthetic reaction centers.

One of my important contribution to the field has been the implementation of a fully quantum version of the ET rate constant using Kubo's generating function theory. This methodology has been further applied to the study of ET rates between chlorophyll-type and quinone-type molecules, and in bulk hetero-junctions.

I have also developed and implemented a second order cumulant theory to compute the rate of ultrafast electron transfer processes in the general case in which the electronic coupling depends on the nuclear coordinates. (Borrelli and Peluso, *J. Chem. Theory Comput.* 2015) The methodology has been applied to predict ET rates in phostosynthetic reactions ceters.

- **Solar energy storage and Photocatalytic water splitting**

  My research activity in this field is dedicated to the development of elementary theoretical models which allows to fully understand the complex photosynthetic mechanisms which takes place in bacteria and plants.

  I have developed several models of potential energy surfaces (PES) for proton-coupled electron transfer (PCET) reactions which are the fundamental steps at the basis of the photosynthetic processes.

  The research is done in collaboration with the group of Prof. Wolfgang Domcke at the Technische Universität München (photocatalytic water splitting), and Prof. Andrea Peluso at the University of Salerno (artificial photosynthesis).

Torino, 15/2/2023

Signature