Francesco Di Maiolo

Curriculum Vitae

Education

2009–2012 **Bachelor of Science**, *Chemistry*, Parma University, Italy.
110/110 with honors, with a theoretical thesis entitled "Real-time vibrational spectroscopy". Supervisor: Prof. Anna Painelli.

2012–2014 **Master of Science**, *Chemistry*, Parma University, Italy.
110/110 with honors, with a theoretical thesis entitled "Electron transfer and magnetism: an exploratory study". Supervisor: Prof. Anna Painelli.

2014–2018 **Ph.D.**, *Chemical Sciences*, Parma University, Italy.
"Summa cum laude", with a dissertation entitled "From Molecules to Materials: Static and Dynamic Properties of Complex Systems". Supervisor: Prof. Anna Painelli.

Research Experience

2014 **Research Fellow**, with Prof. Francesca Terenziani, Parma University, Italy.

2018–2019 **Postdoctoral Fellow**, with Prof. Anna Painelli, Parma University, Italy.

2019 **Postdoctoral Fellow**, with Prof. Irene Burghardt, Institute of Physical and Theoretical Chemistry, Goethe University Frankfurt, Germany.

2020–2022 **Alexander von Humboldt Postdoctoral Fellow**, with Prof. Irene Burghardt, Institute of Physical and Theoretical Chemistry, Goethe University Frankfurt, Germany.

2022–present **Researcher (ricercatore a tempo determinato A - RTDA)**, Parma University, Italy.

Prizes and Grants

- **Alexander von Humboldt postdoctoral fellowship**, total amount: 64,080 €.
- **Italian Chemical Society "Prize for the best scientific paper 2020"**, with motivation "For the distinct contribution to the development of a theoretical method aimed at studying the phenomena of resonant energy transfer as a tool for characterizing the dynamics of photoexcited states in the presence of dynamic disorder" as relevant to the paper Phys. Chem. Chem. Phys. 22, 1061-1068 (2020) "Dynamical disorder and resonance energy transfer: a novel quantum-classical approach".
- **Focus line A/B "Promotion of independent grant proposals"**, awarded by the Goethe Research Academy for Early Career Researchers (GRADE), Goethe University Frankfurt (September 2021), to support the preparation of independent grant proposals (e.g., ERC Starting grant) through proposal workshops, expert instructors and support by an academic mentor during the application phase.

Research interests

Di Maiolo is interested in both method development and applications in three main areas:

1) Magnetic and electric properties in condensed matter organic systems characterized by highly interacting electrons delocalized on deformable crystal lattices, described by means of modified/extended Hubbard and Peierls-Hubbard models;
2) Non-adiabatic dissipative dynamics in photoexcited organic systems (single molecules, dimers and oligomers) by means of both quantum and quantum-classical hybrid approaches. Among them, Di Maiolo uses the Ehrenfest approach, Bloch equation, non-secular Redfield equation, Quantum-Classical Liouville Equation (QCLE), Quantum-Classical Hydrodynamic (Navier-Stokes) equations, Multi-Layer Multi-Configuration Time-Dependent Hartree approach (ML-MCTDH), Multi-Layer Gaussian-based Multi-Configuration Time-Dependent Hartree approach (ML-GMCTDH);
3) Electronic structure calculations on chromophores for OLED applications. Di Maiolo has developed his own code for running truncated configuration interaction (CI) over a class of multiresonant TADF dyes described in terms of the Pariser-Parr-Pople model.

Scientific publications (*=corresponding author)

1 Sissa, C.; Delchiaro, F.; Di Maiolo, F.; Terenziani, F.; Painelli, A.* Vibrational Coherences In Charge-Transfer Dyes: A Non-Adiabatic Picture *J. Chem. Phys*, 141, 164317 (2014).

2 Di Maiolo, F.; Sissa, C.; Painelli, A.* Combining intra- and intermolecular charge-transfer: a new strategy towards molecular ferromagnets and multiferroics *Scientific Reports*, 6, 19682 (2016).

3 Di Maiolo, F.; Masino, M.; Painelli, A.* Terahertz-pulse driven modulation of electronic spectra: Modeling electron-phonon coupling in charge-transfer crystals *Phys. Rev. B*, 96, 075106 (2017).

4 Di Maiolo, F.; Painelli, A.* Intermolecular Energy Transfer in Real Time *J. Chem. Theory Comput.*, 14, 5339-5349 (2018). (**COVER PAPER**)

5 Anzola, M.; Di Maiolo, F.; Painelli, A.* Optical spectra of molecular aggregates and crystals: testing approximation schemes *Phys. Chem. Chem. Phys.*, 21, 19816-19824 (2019).

6 Di Maiolo, F.; Painelli, A.* Dynamical disorder and resonance energy transfer: a novel quantum-classical approach *Phys. Chem. Chem. Phys.*, 22, 1061-1068 (2020).

7 Phan Huu, D. K. A.; Dhali, R.; Pieroni, C.; Di Maiolo, F.; Sissa, C.; Terenziani, F.; Painelli, A.* Antiadiabatic View of Fast Environmental Effects on Optical Spectra *Phys. Rev. Lett.*, 124, 107401 (2020).

8 Di Maiolo, F.*; Brey, D.; Binder, R.; Burghardt, I.* Quantum dynamical simulations of intra-chain exciton diffusion in an oligo (para-phenylene vinylene) chain at finite temperature *J. Chem. Phys.*, 153, 184107 (2020).

9 Di Maiolo, F.; Worth, G. A.; Burghardt, I.* Multi-layer Gaussian-based multi-configuration time-dependent Hartree (ML-GMCTDH) simulations of ultrafast charge separation in a donor–acceptor complex *J. Chem. Phys.*, 154, 144106 (2021).

10 Giavazzi, D.; Di Maiolo, F.; Painelli, A.* The fate of molecular excited states: modeling donor–acceptor dyes *Phys. Chem. Chem. Phys.*, 24, 5555-5563 (2022).

11 Giavazzi, D.; Saseendran, S.; Di Maiolo, F.*; Painelli, A. A Comprehensive Approach to Exciton Delocalization and Energy Transfer *J. Chem. Theory Comput.*, 19, 2, 436-447 (2023). (**COVER PAPER**)

12 Swathi, K.; Sujith, M.; Divya, P. S.; Varghese P, M.; Delledonne, A.; Phan Huu, D. K. A.; Di Maiolo, F.; Terenziani, F.; Lapini, A.; Painelli, A.; Sissa, C.*; Thomas K. G.* From symmetry breaking to symmetry swapping: is Kasha's rule violated in multibranched phenyleneethynylenes? *Chem. Sci.*, 14, 1986-1996 (2023).

13 Crovini, E.; Dhali, R.; Sun, D.*; Matulaitis, T.; Comerford, T.; Slawin, A. M. Z.; Sissa, C.; Azzolin, F.; Di Maiolo, F.; Painelli, A.*; Zysman-Colman, E.* Molecular geometry and the photophysics of thermally activated delayed fluorescence: the strange case of DMAC-py-TRZ *J. Mater. Chem. C*, doi:10.1039/D2TC05213J (2023).

14 Giavazzi, D.; Schumacher, M.; Grisanti, L.; Anzola, M.; Di Maiolo, F.; Zablocki, J.; Lützen, A.; Schiek, M.*; Painelli, A.* A Marvel of Chiral Squaraine Aggregates: Chiroptical Spectra beyond the Exciton Model *J. Mater. Chem. C*, doi:10.1039/D2TC05555D (2023).

15 Bardi, B; Giavazzi, D.; Iagatti, A.; Ferrari, E.; Di Donato, M.; Phan Huu, D. K. A.; Di Maiolo, F.; Sissa, C.; Masino, M.; Lapini, A.*; Painelli, A.* Solid State Solvation: a fresh view *Mater. Horiz.*, doi:10.1039/D3MH00988B (2023).

16 Bedogni, M.; Giavazzi, D.; Di Maiolo, F.*; Painelli, A. Shining light on inverted singlet-triplet emitters *J. Chem. Theory Comput.*, DOI:10.1021/acs.jctc.3c01112 (2023). (**COVER PAPER**)

Invited talks

1 Dynamical Disorder and Resonance Rnergy Transfer: a Novel Quantum-Classical Approach, Virtual Simposium on Chemical Theory and Computation (VS-CTC), online event, December 21, 2020;

2 Quantum Molecular Dynamics in Out of Equilibrium Environments: Redfield-Smoluchowski and Hydrodynamic Approaches, Mathematics Department, University of Surrey, Guildford (UK), October 5, 2022;

3 Harvesting triplet excitons in TADF emitters with negative singlet-triplet gap: The path towards highly efficient OLEDs, Institut fuer Physikalische und Theoretische Chemie, Goethe University Frankfurt, Frankfurt, August 1, 2023.

Contributed talks

1 Di Maiolo, F.; Masino, M.; Painelli, A. ET-F2TCNQ: vibrationally pumped optical spectra, OP2017: 12th International Conference on Optical Probes of Organic and Hybrid Semiconductors, Québec City, Canada, June 19-23, 2017.

2 Di Maiolo, F.; Pieroni, C.; Painelli, A. Intermolecular Energy Transfer in Real Time, XXVI National Congress of the Italian Chemical Society (SCI 2017), Paestum, Italy, September 10-14, 2017.

3 Di Maiolo, F.; Painelli, A. Intermolecular energy transfer in real time, PPES 2018, Pisa, Italy, June 24-27, 2018.

4 Di Maiolo, F.; Painelli, A. Intermolecular energy transfer in real time, WIVACE 2018 XIII Workshop on Artificial Life and Evolutionary Computation, Parma, Italy, September 10-12, 2018.

5 Di Maiolo, F.; Burghardt, I. Theoretical Approaches to Quantum Molecular Dynamics in Out of Equilibrium Environments, WE-Heraeus-Seminar: Koopman Methods in Classical and Classical-Quantum Mechanics, online event, April 19-23, 2021.

6 Di Maiolo, F.; Burghardt, I. Quantum molecular dynamics in out of equilibrium environments: Redfield-Smoluchowski and hydrodynamic approaches, CECAM-FR-MOSER Flagship Workshop "Nonequilibrium dynamical solvent effects on excited states: from spectroscopy to photoreactivity", online event, June 14-17, 2021.

7 Di Maiolo, F.; Burghardt, I. Quantum molecular dynamics in out of equilibrium environments: Redfield-Smoluchowski and hydrodynamic approaches, CT4OPTO Workshop "Principles of light-induced charge transfer for optogenetics", online event, June 14-16, 2021.

8 Di Maiolo, F.; Burghardt, I. Theoretical Approaches to Quantum Molecular Dynamics in Out of Equilibrium Environments, XXVII National Congress of the Italian Chemical Society (SCI 2021), online event, September 14-23, 2021.

9 Di Maiolo, F.; Dhali, R.; Saseendran, S.; Phan Huu, D. K. A.; Giavazzi, D.; Sissa, C.; Terenziani, F.; Painelli, A. Organic light emitting devices (OLED): a playground for multidisciplinary research, Italian Conference on Optics and Photonics (ICOP), Trento, Italy, June 15-17, 2022.

10 Crovini, E.; Dhali, R.; Sun, D.; Matulaitis, T.; Comerford, T.; Cordes, D. B.; Slawin, A. M. Z.; Sissa, C.; Azzolin, F.; Di Maiolo, F.; Painelli, A.; Zysman-Colman, E. Understanding Large Dihedral Angle Relaxation of DMAC-py-TRZ: A joint Experimental and Computational Study of TADF Dye, International Conference on the Science and Technology of Synthetic Metals (ICSM), Glasgow, UK, July 17-22, 2022.

11 Di Maiolo, F.; Burghardt, I. Quantum dynamics of exciton transport in semiconducting polymer chains, International Conference on the Science and Technology of Synthetic Metals (ICSM), Glasgow, UK, July 17-22, 2022.

12 Di Maiolo, F.; Bedogni, M.; Painelli, A. Harvesting triplet excitons in TADF emitters with negative singlet-triplet gap: The path towards highly efficient OLEDs, VII CONGRESSO DELLA DIVISIONE DI CHIMICA TEORICA E COMPUTAZIONALE (DCTC2022), Modena, Italy, September 21-23, 2022.

Posters

1 Sissa, C.; Delchiaro, F.; Di Maiolo, F.; Terenziani, F.; Painelli, A. Vibrational Coherences In Multipolar Dyes: A Non-Adiabatic Approach, 3rd Italian Meeting on Raman Spectroscopy and Non-Linear Optical Effects, Parma, Italy, June 9-11, 2014.

2 Sissa, C.; Delchiaro, F.; Di Maiolo, F.; Terenziani, F.; Painelli, A. Vibrational Coherences In Multipolar Dyes: A Non-Adiabatic Approach, Indo-Italian Meeting – Light on Molecular Functional Materials, Bangalore, India, March 10-11, 2015.

3 Di Maiolo, F.; Agazzi, S.; Painelli, A. Combining Intra & Intermolecular Charge-Transfer: MPTTF-PTM, A New Segregated Stack, School and Workshop on Strongly Correlated Electronic Systems – Novel Materials and Novel Theories, Abdus Salam International Centre for Theoretical Physics, Miramare, Trieste, Italy, August 10-21, 2015.

4 Di Maiolo, F.; Painelli, A. ET-F_2TCNQ: vibrationally pumped optical spectra, 21st ETSF Workshop on Electronic Excitations: dynamics and spectroscopy of correlated systems, Eden University, Lund, Sweden, September 20-23, 2016.

5 Di Maiolo, F.; Painelli, A. ET-F_2TCNQ: vibrationally pumped optical spectra, 8th European Symposium on Computing π-Conjugated Compounds (C-π-C 2017), Malaga, Spain, January 27-28, 2017.

6 Di Maiolo, F.; Painelli, A. ET-F_2TCNQ: vibrationally pumped optical spectra, Molecular Properties and Computational Spectroscopy: from Esoteric Effects to Novel Probing Tools (MPCS 2017), Pisa, Italy, April 10-12, 2017.

7 Di Maiolo, F.; Masino, M.; Painelli, A. ET-F_2TCNQ: vibrationally pumped optical spectra, Nano2Fun Final Conference, Parma, Italy, May 10-12, 2017.

8 Pieroni, C.; Di Maiolo, F.; Painelli, A. Intermolecular Energy Transfer in Real Time, Nano2Fun Final Conference, Parma, Italy, May 10-12, 2017.

9 Di Maiolo, F.; Painelli, A. Intermolecular Energy Transfer in Real Time, Conference on the Complex Interactions of Light and Biological Matter: Experiments meet Theory, Abdus Salam International Centre for Theoretical Physics, Miramare, Trieste, Italy, May 21-25, 2018.

10 Di Maiolo, F.; Painelli, A. Intermolecular Energy Transfer in Real Time, QuEBS 2018: Workshop on Quantum Effects in Biological Systems, Vilnius, Lithuania, July 10-13, 2018.

11 Di Maiolo, F.; Burghardt, I. Quantum Molecular Dynamics in Out of Equilibrium Environments: Redfield-Smoluchowski and Hydrodynamic Approaches, 57th Symposium on Theoretical Chemistry (STC 2021), online event, September 20-24, 2021.

12 Di Maiolo, F.; Burghardt, I.; Painelli, A. Quantum Molecular Dynamics in Out of Equilibrium Environments: Redfield-Smoluchowski and Hydrodynamic Approaches, XXVI Convegno Nazionale di Fisica Statistica e dei Sistemi Complessi, Parma, Italy, June 20-22, 2022.

13 Di Maiolo, F.; Burghardt, I.; Painelli, A. Quantum Molecular Dynamics in Out of Equilibrium Environments: Redfield-Smoluchowski and Hydrodynamic Approaches, XLVIII Congresso Nazionale di Chimica Fisica, Genova, Italy, July 4-7, 2022.

14 Di Maiolo, F.; Bedogni, M.; Painelli, A. Harvesting triplet excitons in TADF emitters with negative singlet-triplet gap: The path towards highly efficient OLEDs, XLVIII Congresso Nazionale di Chimica Fisica, Genova, Italy, July 4-7, 2022.

15 Di Maiolo, F.; Bedogni, M.; Giavazzi, D.; Painelli, A. Shining light on inverted singlet-triplet emitters, 13th International Conference on Excitonic and Photonic Processes in Condensed Matter and Nano Materials (EXCON23), Santa Fe, New Mexico, USA, October 23-26, 2023.

Editor and Referee activity

- Member of the Editorial Board of Frontiers in Chemistry. In particular, Di Maiolo is Review Editor for the Theoretical and Computational Chemistry specialty section of Frontiers in Chemistry.
- Referee for the following journals:
  - Journal of Materials Chemistry C (JMCC);
  - Journal of Chemical Theory and Computation (JCTC);
  - Physical Chemistry Chemical Physics (PCCP);
  - The European Physical Journal B (EPJB).

Teaching

- Chemistry bachelor's degree course "Energia e transizione ecologica, oltre i miti la scienza" (2022-2023, Settore scientifico disciplinare Chimica fisica (CHIM/02)) at Parma University, Parma, Italy. Di Maiolo is "docente titolare del corso".
- Materials Science bachelor's degree course "CHIMICA FISICA DEI MATERIALI CON LABORATORIO" (2022-2023, Settore scientifico disciplinare Chimica fisica (CHIM/02)) at Parma University, Parma, Italy. Di Maiolo is "codocente del corso" together with Cristina Sissa and Anna Painelli.
- Master's degree course "Aktuelle Themen der Physikalischen und Theoretischen Chemie" (Wintersemester, 2020-2021, exercise sessions & exams) at Goethe University, Frankfurt am Main.
- "Cultore della Materia" Settore Scientifico-Disciplinare CHIM/02 at Parma University. Thanks to this title, Di Maiolo was a member of the commission for Physical Chemistry exams from July 2018 to September 2019.
- Di Maiolo has supervised 3 Bachelor's thesis in Chemistry.

Additional activities

- Secondment from March 7, 2015 till April 5, 2015 at the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India, to study, under the guidance of Prof. Swapan K. Pati, the Density Matrix Renormalization Group (DMRG) algorithm.

- Secondment from February 6, 2016 till June 7, 2016 at the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India, to develop, under the guidance of Prof. Swapan K. Pati, a version of the Time-dependent Density Matrix Renormalization Group (tDMRG) algorithm.
- Representative of Chemistry and Material Science PhD students within the Chemistry Department Council at Parma University (from 2014 to 2015).
- Representative of Chemistry PhD students in the Teaching Board of the graduate school in Chemical Sciences at Parma University (from 2014 to 2017).
- Co-supervisor for several students of the Bachelor's and Master's degree in Chemistry at Parma University (from 2014 to 2019).
- Tutor activity for Chemistry undergraduate students at Parma University (from 2015 to 2016).
- Assistance activity within the "Physical Chemistry laboratory 2" course at Parma University (from 2015 to 2017). Total: 24 hours.
- Assistance activity in "Scientific Degrees Project" laboratories for High School students, at the Chemistry Department, Parma University (summer 2015 and summer 2016). Total: 24 hours.
- Assistance activity at "Researchers' Night", Chemistry Department, Parma University, September 25, 2015 and September 30, 2022. Total: 8 hours.
- Outreach activities within the "International Year of Light" at Parma University:
  1. Assistance within the project "Light laboratories", at IMEM-CNR, Parma, Italy, October 19 - November 13, 2015. Total: 2 hours.
  2. Guide at the "Light Exhibition", at Palazzo del Governatore, Parma, Italy, October-December 2015. Total: 8 hours.
  3. Assistance within the project "Project Light and Colors", at Scuola Secondaria di Primo Grado "Vianello", Fidenza, Italy, January 2016. Total: 2 hours.

- Outreach activities organized by Parma University within the "Researchers@School" project at:
  1. Scuola Guatelli, Collecchio, Italy, November 3, 2022. Total: 4 hours.
  2. Scuola Zani, Fidenza, Italy, November 10, 2022. Total: 4 hours.
  3. Scuola Romagnosi, Parma, Italy, November 17, 2022. Total: 4 hours.

- Member of the organizing committee for the International Researchers Night 2023, SCVSA Department, Parma University.

November 15, 2023 Francesco Di Maiolo

In compliance with the DPR 445/2000, I declare, to the best of my knowledge, that all the information reported in this document is true. In compliance with the Italian legislative Decree no. 196 dated 30/06/2003, I hereby authorize you to use and process my personal details contained in this document.