PERSONAL INFORMATION FEDERICO TOTTI

[redacted]

federico.totti@unifi.it

https://www.lamm.unifi.it/vp-184-federico-totti.html

Enterprise	University	EPR
☐ Management Level	☐ Full professor	☐ Research Director and 1st level Technologist / First Researcher and 2nd level Technologist
☐ Mid-Management Level	☒ Associate Professor	☐ Level III Researcher and Technologist
☐ Employee / worker level	☐ Researcher and Technologist of IV, V, VI and VII level / Technical collaborator	☐ Researcher and Technologist of IV, V, VI and VII level / Technical collaborator

RESEARCH ACTIVITY

01/01/1995 – today **Research activity**

Member of the Research Group "Laboratory of Molecular Magnetism" (LaMM) previously directed by Prof. Gatteschi and now by Prof. Sessoli and Prof. Caneschi. Since 2008, FT is the line manager research related to the computational characterization of magnetic and non-magnetic systems, for the molecular, crystalline and hybrid (surface) scenario.

Research interests

- Application of molecular orbital theory in the Hartee-Fock and Kohn-Sham approximation for the study of reaction mechanisms of transition metal compounds in the gas-phase or on surface.
- Using QM/MM approaches for the description of the reaction mechanisms in proteins containing transition metals
- Using approaches post-HF and DFT for the description of excited states and magnetic interactions in poly-nuclear complexes containing organic radicals and / or metals of the First and Second Series of Transition, as well as Lanthanides
- Structural Characterization and Interpretation of Magneto-Spectroscopic Properties of Polynuclear Complexes containing Transition Metals of the First and Second Series by structural and magnetic experimental characterization
- Development of Force Fields is for Isolated and Extended Systems
- Characterization by periodic DFT methods of structural, electronic, and magnetic interactions between surfaces and magnetic substrates
- Applications of the *ab initio* molecular dynamics for the study of the adsorption process of corrosion inhibitors on surfaces and their electronic and thermodynamic parameters
- Use of multi-scale approach for the study of relaxation mechanisms in molecular magnets
- Use of in silico approaches to rationalize structure and electronic properties of complex systems

Research production & its quality

- **100** accepted papers on international journals, **1** book chapter, **2** conference proceedings.

- **Total citations =** *5594* (Google Scholar); *4810* (Scopus); *4691* (WoS); *5321* (ResearchGate)
- **h-index =** *40* (Google Scholar); *37* (Scopus); *37* (WoS): *38* (ResearchGate)
- **Average IF per publication (from 1995 to 2025)**: *8.00 (excluding the book chapter)*
- **Average citations per publication (from 1995 to 2025)**: *55.9* (Google Scholar); *48.1* (Scopus)*, 46.9* (WoS)*, 53.2* (ResearchGate)
- **Publications as Corresponding Author:** *35 (published), 2 (to be submitted)*

- **"Excellent and relevant**" the quality of FT's research for VQR 2004-2010, VQR 2011-2014, VQR 2015-2019, VQR 2020-2024.

- **Qualified as Associated Professor (ASN 2012)**
  • 03/A2 - Models and Methods for Chemical Sciences
  • 03/B1 - Fundamentals of Chemical Sciences and Inorganic systems
  • 03/B2 - Fundamentals of Chemical Technologies
- **Qualified as Full Professor (ASN 2016)**
  • 03/B1 - Fundamentals of chemical sciences and inorganic systems
  • 03/B2 - Fundamentals of chemical technologies
- **Qualified as Full Professor (ASN 2022)**
  • 03/B1 - Fundamentals of chemical sciences and inorganic systems
  • 03/A2 - Models and Methods for Chemical Sciences
- **Eligible for ASN Commissary (all three threshold values) (ASN 2021-23)**
  • n° of papers in the last 10 yrs: **61** vs. *43* (03/A2) *53* (03/B1) 41 (03/B2)
  • n° of citations in the last 15 yrs: **3737** vs. *1370* (03/A2) *1663* (03/B1) 1110 (03/B2)
  • H-index for the last 15 yrs: **30** vs. *21* (03/A2) *23* (03/B1) 20 (03/B2)

Scientific responsibility for international and national research projects, admitted to the funding on the basis of competitive tenders that include peer review

As Principal Investigator (see details in the specific file)

- **9 Projects (national and European):** 1 ISCRA-A, 4 ISCRA-B, 2 DECI, 1 PRACE, and 1 PNRR for total budget above 650K euro

As Unit responsible

- **1 Project (national):** 1 PRIN (96K euro)

As Partecipant (see details in the specific file)

- **23 Projects (national and European):** among them 1 ERC (starting grant), 2 ERC (advanced grant), 1 ERC (synergy grant), 2 DECI, 8 PRIN, 2 FET, 1 QUNATERA, 2 FIRB, 1 COST, 1 Network of Excellence

National and International Collaborations

Past and actual most important collaborations:

- ITALY
  V. Barone, Scuola Normale Superiore di Pisa
  Al. Bencini, D. Gatteschi, R. Sessoli, A. Caneschi, L. Sorace, M. Mannini, L. Messori, An. Bencini, A. Bianchi, A. Scozzafava, **G. Cardini, and M. Pagliai**, Università degli Studi di Firenze
  A. Cornia, Università di Modena e Reggio Emilia
  A. L. Brambilla, Politecnico di Milano
  P. Fantucci, Università Milano-Bicocca
  F. Buonocore, M. Celino, ENEA
  S. Carretta, University of Parma
- FRANCE
  B. Gillon, Laboratoire Leon Brillouin, C.E.A, Saclay
  Y. Pontillon, Centre d'Etudes Nucleaires, Grenoble
  K. Bernot, I.N.S.A., Rennes
  P. Sainctavit, C. cartier dit Moulin, Institut de MIneralogie et de Physique del Milieux

Condensés e Institut Pariesien de Chimie Moleculaire
B. Le Guennic, F. Pontilliart, O. Cador, L. Norel, Institut des Sciences Chimiques de Rennes
J-P. Costes, Laboratoire de Chimie de Coordination du CNRS, Toulouse
C. Adamo, I. Ciofini, Chimie Paristech

- UK
  L. Bogani, University of Oxford
  J. A. McCleverty, University of Bristol
  M.D. Ward, University of Sheffield
- AUSTRIA
  S. Müllegger, Johannes Kepler University, Linz
- IRELAND
  S. Sanvito and **A. Lunghi**, Trinity College, Dublin
- SPAIN
  M. Mattesini, Università Complutense di Madrid
- SWITZERLAND
  M. Iannuzzi, Università di Zurich
- GERMANY
  K. Hegetschweiler, Anorganische Chemie, Universitat des Saarlandes, Saarbruken
  S. Loth, Max Planck Institute for Solid State Research, Stuttgart
  E. Bill, Max-Planck-Institut für Chemisce ENRGIEKonversion, Mulheim
  M. Fonin, University of Konstanz, Konstanz
- POLAND
  G. Kamienarz, University A. Mickiewicz
- ROMANIA
  M. Andruh, University of Bucharest
- BRAZIL
  M.A. Novak, Università Federale di Rio de Janeiro
  M.G.F. Vaz, **E.A. Ponzio**, Università Federale Fluminense;
  J.F. Soares, UFPR
- USA
  D. Goldberg, Northwestern University, Evanston, IL.
- INDIA
  G. Rajaraman, IIT Bombay
- NEW ZEELAND
  S. Brooker, University of Otago

Referee Activity (only the most important are reported):

- **Wiley–VCH**
  Angewandte Chemie, Chemistry – An European Journal, Chemistry – An Asian Journal
- **RCS**
  Chemical Communications, Chemical Physics and Physical Chemistry, Nanoscale
- **ACS**
  Journal of American Chemical Society, Inorganic Chemistry, Journal of Chemical Theory and Computation, Langmuir, Journal of Physical Chemistry, ACS Nano
- **Elsevier**
  Chemical Physics Letters, Inorganica Chimica Acta, Surface Science
- **APS**
  Physical Review B, Physical Review Letters
- **Spinger**
  Nature, Nature Communications

Referee Activity for National and European Agencies

Italian

- **ISCRA**, Italian SuperComputing Resource Allocation
- **INSTM**, Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali
- **VQR**, Italian Research Quality Assessment

European

- **PRACE**, Partnership for Advanced Computing in Europe) (CE)
- **COST**, European Cooperation in Science and Technology (CE)
- **HORIZON**, Research and innovation (CE)
- **DFG**, German Research Foundation (DE)

- **UEFISCDI**, The Executive Agency for Higher Education, Research, Development and Innovation Funding (ROM)
- **NCN**, National Science Centre (Narodowe Centrum Nauki) (PL)
- **GCCR**, Czech Science Foundantion (CZ)

Abroad Visiting Activity

02/02/2007 – 14/02/2007 - **Institute of Physics A. Mickiewicz, University of Poznan**, Poznan (POLAND) @ Prof. G. Kamieniarz

08/11/2015 – 22/11/2015 - **Department of Chemistry, Universidade Federal Fluminense**, Niteroi (BRAZIL) @ Prof. M. F. Vaz

DISSEMINATION ACTIVITY

Organization or participation as a speaker at scientific conferences in Italy or abroad

01/1995 – today **Author e co-author** of more than **150** communications national/international conferences and meetings:

- **20** orals (**13** invited) as single author or principal author
- **1** written (invited)
- > **40** orals as co-author
- **9** seminars (invited) in national, European, and international research Institutes

Conferences Organization:

- (**Member of Program Committee**) Minisimposium on “HPC Applications in Physical Sciences: 10th International Conference on Parallel Processing and Applied Mathematics (PPAM 2013)”, Warsaw, (POLAND) from 08-09-2013 to 11-09-2013
- (**Member of Program Committee**) Minisimposium on "HPC Applications in Physical Sciences: 11th International Conference on Parallel Processing and Applied Mathematics (PPAM 2015)”, Krakow (POLAND) from 06-09-2015 to 09-09-2015
- (**Member of Program Committee**) Minisimposium on "HPC Applications in Physical Sciences: 12th International Conference on Parallel Processing and Applied Mathematics (PPAM 2017)", Lublin, (POLAND) from 11-09-2017 to 13-09-2017
- (**Member of Program and Organization Committees**) 7th European Conference on Molecular Magnetism (ECMM), Florence, (ITALY). Chair of the Poster Session, from 15-09-2019 to 18-09-2019
- (**Co-Chair**) MAGNET 2021: 7th Italian Conference on Magnetism (virtual mode) from 11-02-2021 to 12-02-2021
- (**Co-Chair**) MAGNET 2022: 7th Italian Conference on Magnetism from 09-02-2022 to 11-02-2022
- (**Member of Program Committee**) Minisymposium on “HPC Applications in Physical Sciences: 15th International Conference on Parallel Processing and Applied Mathematics (PPAM 2024)”, Ostrava, Czech Republic, from 8-9-2024 to 11-9-2024
- (**Member of Scientfic Committee**) XXII Brazilian Meeting on Inorganic Chemistry (BMIC), X Latin American Meeting on Biological Inorganic Chemistry (LABIC), XI Brazilian Meeting on Rare Earths (BMRE), and the IV Workshop on Theoretical Bioinorganic Chemistry (WTBC) in 2026

As Speaker:

- **(Oral Communication)** Bencini, I. Ciofini, E. Giannasi, M. Mattesini, F. Totti, V. Barone, G. Capecchi, and A. di Matteo, P. Fantucci, "Density Functional Theory as a Computational Tool of the Multiplet Structure in Molecular Magnetic Systems", III Covegno "Verso la complessità molecolare: modelli per la dinamica ed i processi reattivi", Vico Equense (ITALY) from 26-06-1997 to 28-06-1997
- **(Oral Communication)** F. Totti, A. Bencini, V. Barone and M. Mattesini, "DFT Calculations of Spin Coupling and Electron Delocalization Effects in Di-mu-oxo Bridged Manganese Complexes", 8th International Conference on the Applications of Density Functional Theory to Chemistry and Physics, Roma (ITALY) from 06-09-1999 to 10-09-1999
- **(Oral Communication)** F. Totti, A. Bencini, D. Gatteschi, "DFT as a fundamental tool in the understanding of the magnetic interactions from the molecule to the periodic structure", Workshop "Theoretical Concepts and Techniques for Spin Clusters and Single Molecule Magnets", Firenze (ITALY) from 17-11-2000 to 19-11-2000
- (**Invited Seminar, Prof. Affronte**) F. Totti, "On the calculations of the Exchange Coupling constants on polynuclear transition metal clusters: the spin delocalization problem", INFN-CNR, Modena (ITALY) on 21-06-2005
- (**Invited Seminar, Dr. A. Ferretti and Prof. V. Barone**) F. Totti, "Valenza Mista o Tautomeria di Valenza: due facce dello stesso fenomeno", Centro Nazionale delle

Ricerche, ICCOM, Pisa (ITALY) on 02-02-2006

- (**Invited Oral Communication**) A. Bencini and F. Totti, "Is still the Heisenberg Spin Hamiltonian reliable for multi-nuclear paramagnetic clusters?" CECAM Workshop, Models and Theory for Molecular Magnetism, Lyon (FRANCE) from 18-07-2006 to 21-07-2006
- (**Invited Seminar, Prof. G. Kamieniarz**) F. Totti, The Heisenberg spin Hamiltonian: its Origin and its "Qualitative" Picture, Institute of Physics A. Mickiewicz, University of Poznan, Poznan (POLAND) on 07-02-2007
- (**Invited Seminar, Prof. G. Kamieniarz**) F. Totti, "The Heisenberg spin Hamiltonian: a "Quantitative" Picture", Institute of Physics A. Mickiewicz, University of Poznan, Poznan (POLAND), 2/2007 on 10-02-2007
- (**Invited Seminar, Prof. G. Kamieniarz**) F. Totti, "How is the effective Heisenberg spin Hamiltonian reliable for multi-nuclear paramagnetic clusters?", Institute of Physics A. Mickiewicz, University of Poznan, Poznan (POLAND) on 13-02-2007
- (**Invited Oral Communication**) A. Bencini, G. Rajaraman, F. Totti, M. Tusa, "Modeling Thiols on Au(111): A Possible Route to the SAM of SMMs. Structural, Thermodynamic, and Magnetic Properties of Simple Radicals", Para 2008, Minisymposium on HPC Applications: Molecular Nanomagnet Simulations, Trondheim (NORWAY) from 13-05-2008 to 16-05-2008
- (**Invited Oral Communication**) F. Totti, "The Structure, Energetics and Magnetic properties of alkylthiols and nitronyl nitroxide radical thiols on Au(111): A density functional Theory exploration", SAMIC 2009: Syntheses and Methodologies in Inorganic Chemistry, Bressanone (ITALY) from 30-11-2009 to 03-12-2009
- (**Invited Written Communication**) P. Kozłowski, M. Antkowiak, G. Kamieniarz, A. Mickiewicz, R.E.P. Winpenny, F. Totti, "Magnetic properties of frustrated and anisotropic chromium-based molecular rings and of SMM Fe4 adsorbed on Au(111)", DEISA PRACE Symposium, Helsinki (FINLAND) from 13-04-2011 to 14-04-2011
- (**Invited Oral Communication**) F. Totti, "Sul calcolo delle costanti di scambio in cluster polinucleari di metalli di transizione: da semplici dimeri a sistemi più complessi", WorkShop "Metodi omputazionali per i processi chimici e biochimici", Vignale Monferrato (ITALY) from 10-05-2011 to 13-05-2011
- (**Invited Oral Communication**) F. Totti. "Molecular magnets: the long trip from isolated clusters to self-assembled-monolayers: The anchoring issue and the surface effect on magnetic properties", CECAM workshop "Density Functional Theory (DFT) and Wave Function Theory (WFT) for molecular magnetism", Toulouse (FRANCE) from 20-06-2011 to 22-06-2011
- (**Invited Oral Communication**) F. Totti, "Towards future devices: P-DFT simulations of SMM on Manganites and Gold", II WorkShop: Metodi computazionali per i processi chimici e biochimici, Vignale Monferrato (ITALY) from 22-05-2012 to 25-05-2012
- (**Invited Oral Communication**) F. Totti, "Molecular Magnets on Surfaces: from tailoring to the catwalk", Workshop "Functional Molecules on Surfaces: New Building Blocks for Nano-spintronics", Bonn (GERMANY) from 02-10-2012 to 04-10-2012
- (**Invited Oral Communication**) F. Totti, A. Lunghi, S. Ninova, "Molecular magnets on surfaces: an overview", III Tutorial CP2K, CECAM (Centre Européen de Calcul Atomique et Moléculaire), Zurich (SWITZERLAND) from 16-06-2013 to 22-06-2013
- (**Oral Communication**) G. Fernandez Garcia, A. Lunghi, S. Ninova, R. Sessoli, F. Totti, "Characterization of Molecular Magnets on Surfaces by DFT: $[Fe_4(Ph\text{-}C(CH_2O)_3)_2(dpm)_6]$ on Au(111) and LSMO", Workshop "Functional metalorganics and hybrids", Bad Honnef, (GERMANY) from 16-11-2014 to 20-11-2014
- (**Invited Seminar, Prof. B. Le Guennic**) F. Totti, "SMM on surfaces: An Overview", Institut des Sciences Chimiques de Rennes - UMR CNRS 6226, Universitè de Rennes 1, Rennes, (FRANCE) on 21-01-2015
- (**Oral Communication**) F. Totti, S. Ninova, R. Sessoli, J.A.J. Burgess, S. Loth, L. Malavolti, V. Lanzilotto, M. Mannini, A. Cornia, "Characterization of Single Molecular Magnets on Surfaces by DFT: [Fe4(Ph-C(CH2O)3)2(dpm)6] on Cu2N", Conferenza "Theory meets the Experiment: molecular nanoscience and applications", University College London, London (UK) from 01-06-2015 to 03-06-2015
- (**Oral Communication**) G. Fernandez, A. Lunghi, S. Ninova, R. Sessoli, and F. Totti, "Characterization of Molecular Magnets on Surfaces by DFT: $[Fe_4(Ph\text{-}C(CH_2O)_3)_2(dpm)_6]$ on Au(111)", 5th EUROPEAN CONFERENCE ON MOLECULAR MAGNETISM (ECMM), Zaragoza (SPAIN) from 06-09-2015 to 10-09-2015
- (**Invited Oral Communication**) F. Totti, S. Ninova "Characterization of Single Molecular Magnets on Surfaces: the key role of the computational method", III WorkShop "Metodi computazionali per i processi chimici e biochimici", Vignale Monferrato (ITALY) from 24-09-2015 to 27-09-2015
- (**Invited Seminar, Prof. M. G. Vaz**) F. Totti, "Characterization of Single Molecular Magnets

on Surfaces: the key role of the computational method", Seminars on New Trends on Material and Nano Science @ Universidade Federal Fluminense, Niteroi (BRAZIL) on 12-11-2015

- (**Invited Seminar, Prof. M. Novak**) F. Totti, "Characterization of Single Molecular Magnets on Surfaces: the key role of the computational method", Universidade Federal do Rio de Janeiro, Rio de Janeiro (BRAZIL) on 18-11-2015
- (**Invited Oral Communication**) F. Totti, "Physisorption, chemisorption and heterogeneous catalysis", Smart Winter School, space-time Multiscale Approaches for Research and Technology, Scuola Normale, Pisa (ITALY) from 25-01-2016 to 29-01-2016
- (**Invited Oral Communication**) F. Totti, A. Lunghi, S. Ninova, G. Fernandez Garcia "Molecular magnets and their journey from isolated clusters to self-assembled-monolayers: the key role of computational methods", Conference "Modern Trends in Molecular Magnetism", Mumbai (INDIA) from 19-05-2016 to 21-05-2016
- (**Invited Seminar, Dr. Buonocore and Dr. M. Celino**) F. Totti, "Playing with Single Molecular Magnets in molecular and surface scenarios exploiting multi-scale techniques", ENEA, Centro Ricerche Casaccia, Rome (ITALY) on 14-03-2017
- (**Invited Oral Communication**) F. Totti, M. Briganti, G. Fernandez Garcia, J. Jung, B. Le Guennic and R. Sessoli, The Importance of Being...DyDOTA "6th European Conference on Molecular Magnetism (ECMM)", Bucharest (ROMANIA) from 27-08-2017 to 01-09-2017
- (**Invited Oral Communication**) F. Totti, "Molecular Magnets as forerunners brick in Spintronics: the HPC breakthrough", Advanced Computing Workshop 2020: HPC and beyond, Bologna (ITALIA) on 22-01-2020
- (**Invited Oral Communication**) F. Totti and M. Briganti, "Characterizing Molecular Magnetic Systems," II Workshop of MaterialWell: Materials Modelling for Material Science (virtual mode) from 28-04-2022 to 29-04-2022
- (**Invited Seminar, Prof. S. K. Singh**) F. Totti, "Elective Affinities: when Molecular Magnets Meet the Surface. From the basics to the application to real systems.", workshop, IIT Hyderabad, Hyderabad (INDIAA) on 14-11-2024
- (**Invited Keynote Oral Communication**) F. Totti, "Elective Affinities: when Molecular Magnets Meet the Surface", Modern Trends in Molecular Magnetism & Spins in Molecular Systems, Bangalore from 05-11-2024 to 08-11-2024

TEACHING ACTIVITY

01/10/2017 – today

Associate Professor CHIM/03

Dept. of Chemistry of Università degli Studi di Firenze (@LaMM, Laboratory of Molecular Magnetism)

▪ Hold courses:

- **STRUTTURA ELETTRONICA E PROPRIETA' MOLECOLARI**, Module A
  3 Credits, master's degree course in CHEMICAL SCIENCES (B088)
  Curriculum CHEMICAL STRUCTURE, DYNAMICS, and REACTIVITY (D20)
- **CHEMISTRY**, Module B
  3 Credits, bachelor's degree course in PHYSICS and ASTROPHYSICS (B030)
- **CHIMICA GENERALE E INORGANICA & STECHIOMETRIA**, (*from 09/2018*)
  6 Credits bachelor's degree course in APPLIED PHARMACEUTICAL SCIENCES and QUALITY CONTROL
- **FONDAMENTI DI CHIMICA PER IL DATA/COMPUTATIONAL SCIENTIST**
  4 Credits, master's degree course in DATA SCIENCE, SCIENTIFIC COMPUTING & ARTIFICIAL INTELLIGENCE (*from 09/2023*)
- **CALCOLO ALTE PRESTAZIONI APPLICATO ALLA CHIMICA INORGANICA**
  2 Credits, master's degree course in DATA SCIENCE, SCIENTIFIC COMPUTING & ARTIFICIAL INTELLIGENCE (*from 09/2023*)

01/09/2009 - 31/08/2017

Aggregate Professor CHIM/03

Dept. of Chemistry of Università degli Studi di Firenze (@LaMM, Laboratory of Molecular Magnetism)

▪ Hold courses:

- **ELECTRONIC STRUCTURE AND MOLECULAR PROPERTIES**, Module A
  3 Credits, master's degree course in CHEMICAL SCIENCES (B088)
  Curriculum CHEMICAL STRUCTURE, DYNAMICS, and REACTIVITY (D20)
- **CHEMISTRY**, Module B (*from 09/2014*)
  3 Credits, bachelor's degree course in PHYSICS and ASTROPHYSICS (B030)

01/09/2006 - 01/09/2015

Researcher (RTI) CHIM/03

▪ Assistant to the courses:

- **LABORATORIO di CHIMICA INORGANICA**,
  Bachelor's Degree course in CHEMISTRY
- **LABORATORIO di CHIMICA** (*only for the AY 2006/07*)
  Bachelor's Degree course in CHEMISTRY

01/03/2000 – 31/08/2006 **Post-Doc CHIM/03**

▪ Didactic Collaboration:

- **CHIMICA**, (for 6 AY, from 2000 to 2005)
  Bachelor's Degree course in ENGINEERING

▪ Contract Professor:

- **Applicazioni Informatiche**, (from 27/05/05 to 31/12/05)
  In Modulo Professionalizzante "Esperto in gestione dei sistemi di qualità nel settore alimentare: valutazione ed audit secondo gli standard IFS e BRC" per la facoltà di Farmacia
- **CHIMICA** (from 15/06/2006 – 24/07/2006)
  In Corso Professionalizzante "Gestione delle discariche" per la facoltà di Ingegneria

MENTOR ACTIVITY

01/01/2008 – today **Tutor of 8 PhD Students:** 1 in Materials Science and Technology and 7 in £Chemical Sciences" (**3 in co-tutorship**: 1 with Univ. Rennes 1, France; 1 with Fluminense Federal University of Rio de Janeiro, Brazil), and one with the University of Otago (New Zealand)

-

01/01/2010 – today **Supervisor of 5 and co-tutor of 3 master's degree theses in "Chemical Sciences"**

01/01/2008 – today **Scientific referent of 4 Post-Docs**

MANAGERIAL ACTIVITY

Management or participation in editorial committees of magazines, editorial series, encyclopaedias and treaties of recognized prestige

24/07/2019 – today
- **Member of the Editorial Board of "Molecules",** an international open-access, peer-reviewed journal of Chemistry. "Molecules" is published online by MDPI. Its 2022 impact factor is 4.6

01/04/2019
- **Member of the Editorial Board of "Qauntum Materials Research (QMR",** an international open-access, peer-reviewed journal of Chemistry. "Molecules" is published online by Hapres (Editor-in-Chief Prof. Ruqian Wu, University of California, Irvine). Closed on 2021 by pandemic reasons.

2018
- **Guest editor** of Magnetochemistry (2.9 IF, MDPI), for the special issue 'Magnetic Lanthanide Complexes'

Institutional, organizational and service activities carried out at national and international higher education and research institutions

31/10/2021 – today

01/11/2024 – today
- **Member of the Academic Senate (elected representative for the Scientific Research Area)**

31/10/2021 – today
- **Scientific Referent and coordinator for the University of Florence for the National Center "HPC, Big Data and Quantum Computing".** FT developed and coordinated the drafting of the entire proposal of the University coordinating more than 50 colleagues (now more than 70)

05/2021 – today
- **Department Referent** to give permission to enrolments in Chemistry and Chemical Sciences courses from foreign students

01/10/2017 – today
- **Member of the Teaching Committee** for the three-year Degree Course in Chemistry

and the master's degree Course in Chemical Sciences

08/11/2019 – today	-	**Member of the "Operational Committee for High Performance Computing Infrastructure"** of the University of Florence which led to the drafting of the technical specifications up to the installation and commissioning of a University HPC infrastructure with more than 4500 CPU cores, different hundreds of GPUs and with 100 Gbit/s Infiniband connection
16/04/2019 – today	-	**Coordinator for the University of Florence** of the cultural and scientific cooperation agreement with the Indian Institute of Technology of Mumbai (India)
26/01/2015 – today	-	**Coordinator for the University of Florence** of the cultural and scientific cooperation agreement with the Institut National des Sciences Appliquées de Rennes (France)
16/02/2015 – today	-	**Coordinator for the University of Florence** of the cultural and scientific cooperation agreement with the Universidade Federal Fluminense (Brazil)
09/2019 – today	-	**Member of Course Coordination Commission** for three-year Degree Course Applied Pharmaceutical Science and Quality Control
06/2021 – today	-	**Referent for the Department of Chemistry "U. Schiff"** for the new master degree course in Data Science, Scientific Computing and Artifical Intelligence
01/11/2010 –.01/11/2013	-	**Member of the Board of the Department of Chemistry "U.Schiff"** of the University of Florence for the share of Permanent Researchers
06/2021 – today	-	**Referent** for the Department of Chemistry "U. Schiff" for the SMART node relating to CECAM (Centre Européen de Calcul Atomique et Moléculaire)
01/10/2010 –.10/10/2014 & 01/03/2018 –.01/10/2021	-	**Member of the Academic Board of the Doctorate** in "Chemical Sciences" at the Department of Chemistry "Ugo Schiff" of the University of Florence

QUALIFICATIONS

10/1996-03/2000	**PhD in "Science and Technology of Materials".** Viva on March 2000: "DFT Modelling of Magnetic Interactions in Molecular Materials" , Università degli Studi di Firenze, ITALY
10/1990-07/1995	**Master's degree in Chemistry.** Thesis on "Characterization and Reactivity of Organomercurial Compounds with Quantomechanical Methods", Università degli Studi di Firenze, ITALY
1996	**Qualification to practice as Chemist** State examination held in Florence, ITALY

PERSONAL SKILLS

Mother tongue(s)	Italian
Other language(s)	English (proficient); French (intermediate); Spanish (basic)