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| **Curriculum Vitae** |  | http://www.dsctm.cnr.it/images/Eventi_img/Giornata_Dip_2019/Premi/Ambrosio/Ambrosio_foto.jpg |

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| Name / Surname |  | Francesco Ambrosio | |
| Address |  | Viale Italia 52, Avellino 83100, Italy | |
| Phone |  | +39 3897851287 |  |
| Fax |  |  | |
| E-mail |  | Francesco.Ambrosio@unibas.it | |

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| Nationality |  | Italian |

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| Date of birth |  | 23-09-1985 |

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| Gender |  | Male |

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| **Interests** |  | **Research: computational and theoretical chemistry, materials science.** |
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| **Work experience** |  | |

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| Dates |  | 2022-current |
| Occupation or position held |  | Researcher (RTDB) |
| Name of employer |  | Università degli Studi della Basilicata |
| Type of business or sector |  | Research institution, University |
| Main activities and responsibilities |  | Research on (i) the electronic properties of organic semiconductors, (ii) heterogeneous photocatalysis Teaching: Physical Chemistry II for undergraduate students. |
| Dates |  | 2022 |
| Occupation or position held |  | Researcher (RTDA) |
| Name of employer |  | Università degli Studi di Salerno |
| Type of business or sector |  | Research institution, University |
| Main activities and responsibilities |  | Research on (i) the electronic properties of acene crystals, (ii) reaction mechanism of nitration of aromatic compounds, (iii) energy levels of DNA bases. Teaching: Physical Chemistry I for undergraduate students. |
| Dates |  | 2019-2021 |
| Occupation or position held |  | Post-doctoral Researcher |
| Name of employer |  | Istituto Italiano di Tecnologia, Università di Perugia |
| Type of business or sector |  | Research institution, University |
| Main activities and responsibilities |  | Research on the electronic properties of lead halide perovskites. |
| Dates |  | 2014-2018 |
| Occupation or position held |  | Post-doctoral Researcher |
| Name of employer |  | École Polytechnique Fédérale de Lausanne |
| Type of business or sector |  | Research institution, University |
| Main activities and responsibilities |  | Research on the electronic properties of liquid water and water/semiconductor interfaces. |

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| Dates |  | June 2010-July 2010 |
| Occupation or position held |  | Substitute teacher |
| Name of employer |  | Liceo Artistico P.A. De Luca |
| Type of business or sector |  | School |
| Main activities and responsibilities |  | External examiner for the final examinations of high school |
| **Education and training** |
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| Dates |  | October 2010-October 2014 |
| Title of qualification awarded |  | Postgraduate certificate for transferable skills in science |
| Principal subjects |  | Team Working in a Research Environment, Communication in Science. |
| Name and type of organisation providing education and training |  | University of Warwick |

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| Dates |  | October 2010-October 2014 |
| Title of qualification |  | PhD – School of Chemistry |
| Principal subjects |  | Computational chemistry, modelling, data analysis.  Degree thesis entitled: “Theoretical studies of the dynamics of electron transfer in dye sensitized solar cells and of the mechanism of singlet fission in organic crystalline materials” |
| Name and type of organisation providing education and training |  | University of Warwick |
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| Dates |  | September 2010 |
| Title of qualification |  | IELTS examination (overall grade 7) |
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| Dates |  | October 2007 - October 2009 |
| Title of qualification awarded |  | Master Degree in “Physical chemisty of complex systems” 110/110 *magna cum laude*  Degree thesis entitled “Microsolvation and spectroscopic properties of the N-Methyl-6-Quinolone in aqueous solution” |
| Principal subjects |  | Physical Chemistry, Computational chemistry and Spectroscopic Methods |
| Name and type of organisation providing education and train**z** |  | Università degli Studi Federico II – Napoli |
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| Dates |  | October 2003 - July 2007 |
| Title of qualification awarded |  | Degree in “Chemistry” 110/110 *magna cum laude*  Degree Thesis entitled “Electroanalytical methods in the study of Metal-Water-Histidine system” |
| Principal subjects |  | Chemistry, Physics, Mathematics |
| Name and type of organisation providing education and training |  | Università degli Studi Federico II – Napoli |

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| Dates |  | September 1998 – June 2003 |
| Title of qualification awarded |  | High School Graduate – 100/100 |
| Name and type of organisation providing education and training |  | Liceo Scientifico P.S. Mancini, Avellino |

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| **Personal skills and competences** |

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| Mother tongue |  | **Italian** |

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| Other language | **English** |
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| Skills and competences |  | Familiar skills with Windows and Linux operative systems. Good usage of FORTRAN programming language; Excellent usage of of the QUANTUM ESPRESSO, CP2K, GAUSSIAN03 and CRYSTAL09 suite of codes. Exstensive experience in DFT and TD-DFT methods for electronic structure calculations. Extensive experience in molecular dynamics simulation methods. Large experience in modelling and in development of theory and methods. |
| **National Scientific Abilitation** |  | I hold the National Scientific Habilitation as Associate Professor in the following classes:  03/A2 - MODELLI E METODOLOGIE PER LE SCIENZE CHIMICHE  03/B1 - FONDAMENTI DELLE SCIENZE CHIMICHE E SISTEMI INORGANICI  03/B2 - FONDAMENTI CHIMICI DELLE TECNOLOGIE |

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| Personal Interests |  | Literature; Theatre; Arts, Martial Arts (20 years of practise). |

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| Driving Licence |  | Car driving licence since February 2005 |

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**Attachments** Prize: Young Investigator Award 2019 ([link](https://www.dsctm.cnr.it/it/conferenza-di-dipartimento-2019.html))

Author of **56** Publications in International Scientific Journals List of publications available at the following link: [Articles](https://scholar.google.com/citations?hl=en&user=ikBvQI0AAAAJ&view_op=list_works)

**SCIENTIFIC PROJECTS**

a) Participation to the NCCR-MARVEL project (http://nccr-marvel.ch/), a centre on Computational Design and Discovery of Novel Materials created by the Swiss National Science Foundation in May 2014. I started working in NCCR-MARVEL soon after its foundation in November 2014 and I participated to this project for 4 years (2014-2018).

b) Participation to the European Union’s Horizon 2020 research and innovation programme under grant agreement no. 764047 of the ESPRESSO project in collaboration with several experimental groups (2020-2022)

c) Participation to the EU project PERTPV, a project aimed at advancing the perovskite thin-film PV technology by improving both efficiency and stability of the perovskites-based devices (2019-2020).

<https://ec.europa.eu/inea/en/horizon-2020/projects/h2020-energy/solar-energy/pertpv>

c) Participation to the ERC project SOPHY, aimed at developing the tools and knowledge to probe optoelectronic processes at buried interfaces, in perovskites opto-electronic devices, at operating conditions (2021-2022)

. <https://sophyerc.eu/team/francesco-ambrosio/>

e) Participation to the project titled: Advanced and sustainable approaches for design and analysis of innovative solid-state electrolytes for next-generation lithium batteries" Acronym: SULDEBAT NEXTGENERATIONEU”, PROGETTO “MOST” SPOKE 13, CUP D43C22001180001

f) Principal investigator of the PRIN 2022 PNRR project titled: DEvising SoLar-driven catalysis at Perovskites Heterogeneous Interfaces (2023-

g) Project PON-GREEN/01CUP: D41B21003760003 in the framework of the REACT-EU DM 1062/2021 funding scheme, focussed on the study of the opto-electronic properties of organic semiconductors to be used in organic solar cells (2022)

h) Principal investigator of a class C project awarded by ISCRA upon peer review titled "Ab initio determination of charge localization in organic semiconductors" , code HP10C4OQ9O (2022-2023)

(i) Principal investigator of a class C project awarded by ISCRA upon peer review titled "Defect Chemistry of Organic Semiconductors from Ab initio Electronic structure" Code: Def-OCS HP10CKGMYR (2023-)

**LIST OF SCIENTIFIC CONFERENCES/WORKSHOPS/EVENTS**

Poster presentation - MC10: International Conference on Materials Chemistry in Manchester, United Kingdom Title of the presentation: Localization of the injected electron in Dye Sensitized Solar Cells: comparison of different theoretical approaches. 04/07/2011 07/07/2011

Poster presentation - ACS National Meeting San Diego, United States of America Title: Effect of the anchoring group on electron injection: Theoretical study of phosphonated dyes for dye-sensitized solar cells <https://www.morressier.com/article/effect-anchoring-group-electron-injection-theoretical-study-phosphonated-dyes-dyesensitized-solar-cells/5fc62e239e0a135cbec74f51>? 25/03/2012 29/03/2012

Poster Presentation - 2nd Thomas Young Centre (TYC) Workshop & Tutorial on Energy Materials: Charge transfer for energy applications , London, United Kingdom Title of the presentation: Modeling the anchoring group for dye-sensitized solar cells: dye structure, attachment chemistry and their effect on electron injection rates. <https://www.thomasyoungcentre.org/events/482/2nd-tyc-energy-materials-workshop-and-tutorial/> 06/06/2012 08/06/2012

Poster Presentation - the 10th International Conference on Excitonic Processes in Condensed Matter, Nanostructured and Molecular Materials, EXCON 2012 Groeningen, The Netherlands Title of the poster presentation: 02/07/2012 06/07/2012

Poster presentation - "Nothing is perfect - the quantum mechanics of defects" , Ascona, Switzerland Title: "Charge transition levels of point defects in crystalline materials through thermodynamic integration" 26/04/2015 29/04/2015

Invited Talk at PSI-K 2015 Conference Donostia/San Sebastian, Spain Title: "Electronic structure and redox levels of liquid water: effect of non local van der Waals interactions and hybrid functionals" 06/09/2015 10/09/2015

Poster Presentation - Marvel Review and Retreat 2016, EPFL, Lausanne, Switzerland Title of the Poster presentation: "Redox levels in aqueous solution and at the semiconductor-water interface: Theory and applications" 08/09/2016 09/09/2016

Invited Talk - 2016 MARVEL Junior Retreat with a presentation entitled “Redox levels in aqueous solution: effect of van der Waals interactions and hybrid functionals” <https://nccr-marvel.ch/events/marvel-junior-retreat-2016> 20/07/2016

Invited Talk - EMRS Fall Meeting in Warsaw, Poland Symposium U "Characterization of advanced materials" Title of the presentation: Redox levels in aqueous solution: effect of non local van der Waals interactions and hybrid functionals"

<https://www.european-mrs.com/computer-modelling-nanoscience-and-nanotechnology-atomic-scale-perspective-iv-emrs> 19/09/2016 22/09/2016

Organizator of Marvel Junior Seminars at EPFL, Lausanne, a series of seminars aimed at intensifying interactions between the MARVEL Junior scientists belonging to different research groups. <http://nccr-marvel.ch/outreach/education-and-training/marvel-junior-seminars>, 01/01/2017 01/11/2018

Contributed Talk - Computational Molecular Science 2017 - 19-22 May 2017 University of Warwick, Coventry, UK Title of the presentation: "Electronic structure of the hydrated electron: a hybrid functional study" 19/05/2017 22/05/2017

Contributed Talk - International Workshop on Computational Electrochemistry Helsinki, Finland Title of the presentation: "pH-dependent surface chemistry and catalytic reaction pathway from first-principles" 09/07/2018 12/07/2018

Contributed Talk - Annual Meeting of the Swiss Physical Society, Lausanne, Switzerland Advanced Electronic-Structure Developments and Applications Title: "pH-dependent surface chemistry and catalytic reaction pathway from first-principles" 28/08/2018 31/08/2018

Contributed Talk - Dipartimento di Scienze e Tecnologie dei Materiali - CNR CONFERENZA DI DIPARTIMENTO 2019, Bressanone, Italy Title of the presentation: "On the electronic properties of metal halide perovskites" 28/10/2019 30/10/2019

Contributed Talk - HOPE-PV202 Chernokogolovka, Russia , Title of presentation: “Charge trapping at the surface of metal halide perovskites” 22/11/2021 25/11/2021

Invited Speaker/Lecturer for the course “NANOMATERIALI E NANOTECNOLOGIE: opportunità e rischi. REACH – CLP” organized by ASL Salerno 13/12/2021

Invited Talk “Modelling, Theory, Simulation” (MoThS), at the Abbaye des Prémontrés in Pont-à-Mousson Section 4- Physics and Chemistry of Solid/Liquid Interfaces Title presentation: Charge localization in metal halide perovskites: effects on photovoltaics and photocatalysis 14/005/2024 16/05/2024

Invited Talk - Università degli Studi di Cagliari in the framework of the PRIN 2022 PNRR project DELPHI Title of Presentation: "Charge localization in semiconductors: effects on photovoltaics and photocatalyisis." 13/06/2024

**TEACHING ACTIVITIES**

1) At EPFL I have fulfilled teaching duties from 2016 to 2018 in the framework of General Physics IV courses for bachelor students As such, I have contributed to several tasks, including:

• Regular meetings with the professor in preparation for the course

• Preparation of materials to be distributed to students

• Coaching in the classrooms : explanation of exercices and assistance for their resolution

• Preparation of review sessions and supervision of students during tests and intermediate examinations

• Correction and evaluation of tests.

2) "Electron transfer in molecules and in condensed phases: Fundamentals and applications” (18h, 3CFU) Corso di dottorato in Scienze Chimiche dell’Università degli Studi di Perugia Dottorandi dei Cicli XXXIII- XXXVI Anno accademico 2019-2020 Course Program: (i) Introduction to electron transfer processes, (ii) Dynamics of electron transfer: the Marcus theory, (iii) Intramolecular and intermolecular charge transfer, (iv) electron tranfer processes in liquid water: redox chemistry in aqueous solution, (v) charge localization in crystalline and amorphous materials (vi) heterogenous charge transfer processes at the interface between different molecules/materials (vii) charge transfer processes in biological systems.01/11/202018/12/2020

3) At “Università degli Studi di Salerno”, I have been assigned to the course of “Physical Chemistry 1”. In particular, I have taught how to solve problems and exercises typically encountered in the application of the principles of quantum mechanics to chemical systems.

4) At “Università degli Studi della Basilicata”, I am currently teaching the course of “Physical Chemistry 2”, “Laboratory of Physical Chemistry 2” and the course of “Physical Chemistry of Materials”.

**Attachments** Prize: Young Investigator Award 2019 ([link](https://www.dsctm.cnr.it/it/conferenza-di-dipartimento-2019.html))

List of publications available at the following link: Articles