

# ACADEMIC PORTFOLIO

SIMONE TAIOLI

## Personal Data

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**Date of birth:** 27/09/1974  
**Place of birth:** Cesena (Italy)  
**Citizenship:** Italian  
**Gender:** Male  
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## Current appointments

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### Senior Research Scientist

European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT\*),  
Strada delle Tabarelle, 286 – Trento, Italy

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## Education and previous academic appointments

### Higher education

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**Oct 2009 – Apr 2013:** 2<sup>nd</sup> PhD in Physics (**Doctor Europaeus**), University of Trento, Trento (IT).

- Second PhD in theoretical condensed matter physics. Final mark: **excellent**.
- Final dissertation: “*From materials science to astrophysics with electronic structure calculations*”.
- Advisor: Prof. Siddharth Saxena (University of Cambridge, UK), Co-advisors: Dr. Stefano Simonucci (University of Camerino, Italy), Dr. Maurizio Dapor (ECT\* & University of Trento, Italy).

**Jan 2001 – May 2004:** 1<sup>st</sup> PhD in Nuclear Science and Technology, University of Bologna (IT) and Scuola Normale Superiore, Pisa (IT)

- **By competition scoring first.**
- Final dissertation: “*Inner shell photoionization and non-radiative decay processes in molecules: theory and calculations*”.
- Advisor: Dr. Stefano Simonucci (University of Camerino, Italy), Co-advisors: Prof. Renato Colle (Scuola Normale Superiore & University of Bologna, Italy) & Prof. Jorge Fernandez (University of Bologna, Italy)

**Oct 1994 – Dec 2000:** Undergraduate student in Nuclear Science and technology, University of Bologna, Bologna (IT).

- Course Duration: 5 years + M.Sc. in Plasma and Reactor Physics: first-class (**summa cum laude - 100/100 e lode**).
- Final dissertation: “*Quantum mechanical calculation of Auger spectra of silicon clusters.*”.
- Advisor: Prof. Renato Colle (Scuola Normale Superiore & University of Bologna, Italy),  
Co-advisor: Dr. Stefano Simonucci (University of Camerino, Italy).

## Previous employment

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**Oct 2022 – Oct 2023** Associate Professor at Gdańsk University of Technology – Gdańsk, Poland

**Sept 2020 – Feb 2022** Adjunct Professor at Peter the Great St. Petersburg Polytechnic University – St. Petersburg, Russia (from 1st Sept 2022 appointed to Full Professor, part-time, I resigned and halted all formal commitments)

**Oct 2015 – Dec 2017** Adjunct Professor at the Institute of Particle and Nuclear Physics, Charles University –Prague (CZ)

**May 2010 – Dec 2014** Tenured position – Solid State and Materials Science **group leader** at the Interdisciplinary Laboratory for Computational Science, Center for Materials and Microsystems, Bruno Kessler Foundation & University of Trento – Trento (IT)

**May 2008 – May 2010** Tenure-track position at the Center for Materials and Microsystems, Bruno Kessler Foundation – Trento (IT)  
*Light-matter interaction for the interpretation of electron spectra.*

**Oct 2007 – Apr 2008** Post-doctoral Research fellow at the Electronic Engineering Department, The University of Sheffield – Sheffield (UK)  
*Excitonic effects in carbon-based nanostructures.*

**Oct 2005 – Sept 2007** Post-doctoral Research fellow at the Earth Sciences Department, University College London – London (UK)  
*DFT and QMC modelling of transition metals*

**Jan 2004 – Sept 2005** Post-doctoral Research fellow at the Physics & Astronomy Department, University College London – London (UK)  
*Time-dependent wave-packet propagation in electron-molecule scattering*

## Military service

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**August 2000 – July 2001** Compulsory military service.

## Academic Habilitations to teach at Italian and European Universities

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- National Scientific Habilitation to Full Professor (prima fascia) in **Theoretical Condensed Matter Physics (SSD 02/B2)**, Italy
- Qualification aux fonctions de Professeur des universités - **Milieux denses et matériaux**, France.

- National Scientific Habilitation to Associate Professor in **Theoretical Condensed Matter Physics (SSD 02/B2)**, Italy
- National Scientific Habilitation to Associate Professor in **Models and Methods for the Chemical Sciences (SSD 03/A2)**, Italy
- Qualification aux fonctions de maître de conférences - **Milieux denses et matériaux**, France.

## Research activity

### Research Interests

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- **Development and application of state-of-the-art many-body techniques**, from mean-field (Hartree-Fock and Density Functional Theory also Time-dependent) to methods beyond mean-field, such as configuration interaction (CI), many-body perturbation theory (GW), Multi-configurational self-consistent approaches (MP2, MCSCF, RASPT2), and Path-Integral Monte Carlo (PIMC).
- **Development and application of theoretical spectroscopy methods** to study resonance-affected photo-excitation events in materials at different scales of aggregation in their interaction with external fields. I am a main developer and maintainer of the SURPRISES code, which is a mixed *ab-initio* and Monte Carlo suite to simulate electron spectra (XPS, Auger, ARPES, EELS, NEXAFS) and vibrational spectra (IR) of organic and inorganic molecules in gas or solid phase.
- **Physics of cancer** Monte Carlo modelling of hadron and proton therapy experiments via *ab-initio* and Monte Carlo methods.
- **Mixed Monte Carlo and ab-initio modeling** of charge transport, secondary emission spectra and yields of solids.
- **Photochemistry and photophysics**: study of light-harvesting systems, such as multi-chromophoric Pigment Protein Complexes, bacteriochlorophyll, carotene, with both multi-reference methods typically used in quantum chemistry to interpret two-dimensional and pump-probe non-linear spectroscopies.
- **Development of novel methods to study  $\beta$ -decay in stellar nucleosynthesis** of evolved stars and in Big-Bang nucleosynthesis. We have implemented from scratch a relativistic approach to scattering theory, based on the Dirac-Hartree-Fock approximation, to interpret the  $\beta$ -decay spectra of heavy nuclei, such as lanthanides (used to develop scintillators for atomic and nuclear physics experiments) and actinides.
- **Materials modelling under extreme conditions of temperature and pressure**, applied particularly to Earth and mineral sciences.
- **Artificial Intelligence for Quantum Systems**: development of Deep Learning solutions for the investigation of quantum states.
- **Modeling of carbon-based nanostructures**, such carbon nanotubes, fullerenes, graphene, graphene foams, nanotubes bundles and of functional, memristive and bio-inspired materials.
- **Ultra-cold Fermi gases at unitarity** and BCS superconductivity.
- **Study of Metal-Organic frameworks (MOF) and Zeolitic Imidazolate framework (ZIF)** for gas separation and storage.
- **Computational modeling of crystal growth.**

## Conference organization

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*5th Topical Meeting on Industrial Radiation and Radioisotope Measurement Applications (IRRMA-V) – 09-14/06/2002, Bologna (IT)*

*New Frontiers in Multiscale Modelling of Advanced Materials – 17-20/06/2014, European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT\*), Trento (IT)*

## Graduate and undergraduate teaching

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- *Density functional approaches to the many-body problem*, 3<sup>rd</sup> year degree in Physics at Gdańsk University of Technology (March - May 2023)
- *Dielectric-response models within an ab-initio framework*, Summer school to PhD students in Physics at Gdańsk University of Technology (July 2023)
- *Scattering of waves and particles*, Summer school to PhD students in Physics at Gdańsk University of Technology (August 2022)
- *Scattering theory*, Winter school to PhD students in Physics at Gdańsk University of Technology (December 2021)
- *Advanced Problems in Condensed Matter Physics*, 5<sup>th</sup> year master degree in Physics, Peter the Great St.Petersburg Polytechnic University, Russia (Sept – Dec 2021)
- *Scattering theory*, PhD in Physics and Engineering at the the Gdańsk University of Technology (June 2021)
- *Advanced Problems in Condensed Matter Physics*, 3<sup>rd</sup> year undergraduate degree in Physics, Peter the Great St.Petersburg Polytechnic University, Russia (Sept – Dec 2020)
- *Scattering theory with applications to Condensed Matter and Nuclear Physics*, 4<sup>th</sup> and 5<sup>th</sup> year physics students, Charles University in Prague (Feb – June 2016)
- *Computational Materials Science*, PhD in Materials Engineering at the University of Trento (March – April 2014)

## Advisory and co-advisory role for undergraduate and graduate students

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I am currently **co-tutoring four PhD students**:

- **Piero Luchi** at the Physics Department, University of Trento along with Prof. F. Pederiva on *Machine Learning techniques FOR Quantum Gate Engineering (ML Q-FORGE)* from 01/11/2019 - to date.
- **Alessandro Piccoli** at the Physics Department, University of Trento along with Prof. A. Miotello on *Quantum sensing with laser-synthesized nano-diamond NV color centers (NADIA)* from 01/11/2020 - to date.
- **Francesco Carnovale** at the Physics Department, University of Trento along with Prof. G. Lattanzi on *4D Microscopy of biological materials by short pulse terahertz sources (MIMOSA)* from 01/11/2022 - to date.
- **Giovanni Novi Inverardi** at the Physics Department, University of Trento along with Prof. G. Lattanzi on *4D Microscopy of biological materials by short pulse terahertz sources (MIMOSA)*

from 01/11/2022 - to date.

I also **officially supervised two PhD students:**

- **Francesco Segatta** at the Chemistry Department, University of Bologna along with Prof. M. Garavelli on *Computational Based Design of Bio-Inspired Electrochromic Molecules for Colour Tunable Electronic Ink* from 01/10/2014 to 17/04/2017. Final mark: Excellent cum laude

### Outcomes

1. **“A quantum chemical interpretation of 2DES spectra of Light-Harvesting complexes”**  
Segatta F. & Cupellini L. & Jurinovich S. & Mukamel S. & Dapor M. & **Taioli S.** & Garavelli M. & Mennucci B.  
J. Am. Chem. Soc. 139 (22), 7558 (2017)
2. **“UV-light induced vibrational coherences, the key to understand Kasha rule violation in trans-azobenzene”**  
Borrego-Varillas R. & Nenov A. & Oriana A. & Omachi J. & Ganzer L. & Manzoni C. & Segatta F. & Conti I. & Segarra-Marti J. & Dapor M. & **Taioli S.** & Mukamel S. & Garavelli M. & Cerullo G.  
J. Chem. Phys. Lett. 9, 1534 (2018)
3. **“Ultrafast Carotenoid to Retinal Energy Transfer in Xanthorhodopsin Revealed by the Combination of Transient Absorption and Two Dimensional Electronic Spectroscopy”**  
Segatta F. & Gdor I. & Julien R ehault J. & **Taioli S.** & Friedman N. & Sheves M. & Rivalta I. & Ruhman S. & Cerullo G. & Marco Garavelli M.  
Chemistry - A European Journal 24, 12084 (2018)

- **Tommaso Morresi** at the Faculty of Mechanical and Environmental Engineering, University of Trento on *Computer simulations of the electronic structure and topological properties of graphene and other 2D materials* from 01/11/2015 to 29/05/2019. Final mark: Excellent

### Outcomes

1. **“Exploring event horizons and Hawking radiation through deformed graphene membranes”**  
Morresi T. & Simonucci S. & Binosi D. & R. Piergallini & Roche S. & Pugno N. & **Taioli S.**  
2D Materials 7, 041006 (2020)
2. **“Structural, Electronic and Mechanical properties of all-sp<sup>2</sup> graphene allotropes with density lower than graphene”**  
Morresi T. & Pedrielli A. & Pugno N. & Gabbrielli R. & a Beccara S. & **Taioli S.**  
Carbon 159, 512 (2020)
3. **“Anisotropic approach for simulating electron transport in layered materials: computational and experimental study of Highly Oriented Pyrolytic Graphite”**  
Azzolini M. & Morresi T. & Stehling N. & Rodenburg C. & Pugno N. & **Taioli S.** & Dapor M.  
J. Phys. Chem. C 122 (18), 10159 (2018)

4. **“A Novel Combined Experimental and Multiscale Theoretical Approach to Unravel the Structure of SiC/SiO<sub>x</sub> Core/shell Nanowires For Their Optimal Design”**  
Morresi T. & Timpel M. & Pedrielli A. & Garberoglio G. & Pasquali L. & Tatti R. & Pugno N. & M.V. Nardi & **Taioli S.**  
Nanoscale 10, 13449 (2018)
5. **“Relativistic theory and ab-initio simulations of electroweak decay spectra in medium-heavy nuclei and of atomic and molecular electronic structure”**  
Morresi T. & **Taioli S.** & Simonucci S.  
INVITED PAPER: Advanced Theory and Simulations Adv. Theory Simul. 1, 1870030 (2018) - JOURNAL COVER
6. **“Monte Carlo simulations of measured electron energy-loss spectra of diamond and graphite: Role of dielectric-response models”**  
Azzolini M. & Morresi T. & Garberoglio G. & Calliari L. & Pugno N. & **Taioli S.** & Dapor M.  
Carbon 118, 299 (2017)

I also closely, even though not officially, supervised further three PhD students:

- **Martina Azzolini** at the Faculty of Mechanical and Environmental Engineering, University of Trento on *Monte Carlo simulations of energy loss and secondary electron spectra of solid targets* from 01/11/2015 to 30/04/2019. Final mark: Excellent

## Outcomes

1. **“Computational tools for calculating REEL spectra in solids: a comparison between Monte Carlo method and the numerical solution of the Ambartsumian-Chandrasekhar equations”**  
Azzolini M. & Ridzel O.Y. & Kaplya P. & Afanas’ev V. & Pugno N. & **Taioli S.** & Dapor M.  
Computational Materials Science 173, 109420 (2020)
2. **“Secondary electron emission and yield spectra of metals from Monte Carlo simulations and experiments”**  
Azzolini M. & Angelucci M. & Cimino R. & Larciprete R. & Pugno N. & **Taioli S.** & Dapor M.  
J. Phys.: Condens. Matter 31, 055901 (2019)
3. **“Anisotropic approach for simulating electron transport in layered materials: computational and experimental study of Highly Oriented Pyrolytic Graphite”**  
Azzolini M. & Morresi T. & Stehling N. & Rodenburg C. & Pugno N. & **Taioli S.** & Dapor M.  
J. Phys. Chem. C 122 (18), 10159 (2018)
4. **“Monte Carlo simulations of measured electron energy-loss spectra of diamond and graphite: Role of dielectric-response models”**  
Azzolini M. & Morresi T. & Garberoglio G. & Calliari L. & Pugno N. & **Taioli S.** & Dapor M.  
Carbon 118, 299 (2017)

- **Dr. Andrea Pedrielli** at ECT\* and at the Faculty of Mechanical and Environmental Engineering, University of Trento on from 01/11/2014 to 30/04/2018

## Outcomes

1. **“Electronic excitation spectra of cerium oxides: from ab initio dielectric response functions to Monte Carlo electron transport simulations”**  
Pedrielli A. & De Vera P. & Trevisanutto P. & Pugno N. & Abril I. & Garcia-Molina R. &

**Taioli S.** Dapor M.

Physical Chemistry Chemical Physics 23, 19173 (2021)

2. **“Designing graphene-based nanofoams with nonlinear auxetic and anisotropic mechanical properties under tension or compression”**

Pedrielli A. & **Taioli S.** & Garberoglio G. & Pugno N.

Carbon 111, 796 (2017)

3. **“Gas Adsorption and Dynamics in Pillared Graphene Frameworks”**

Pedrielli A. & **Taioli S.** & Garberoglio G. & Pugno N.

Micropor. Mesopor. Mater. 257C, 222 (2018)

4. **“The Mechanical and Thermal Properties of Graphene Random nanofoams via Molecular Dynamics Simulations”**

Pedrielli A. & **Taioli S.** & Garberoglio G. & Pugno N.

Carbon 132, 766 (2018)

5. **“A Novel Combined Experimental and Multiscale Theoretical Approach to Unravel the Structure of SiC/SiO<sub>x</sub> Core/shell Nanowires For Their Optimal Design”**

Morresi T. & Timpel M. & Pedrielli A. & Garberoglio G. & Pasquali L. & Tatti R. & Pugno N. & M.V. Nardi & **Taioli S.**

Nanoscale 10, 13449 (2018)

- **Anna Battisti** at the Faculty of Physics, University of Trento on *Computer Simulation of Biological Systems* from 01/11/2010 to 12/03/2013

## Outcomes

1. **“Zeolitic Imidazolate Frameworks for separation of binary mixtures of CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>, and H<sub>2</sub> separation: a computer simulation investigation”**

Garberoglio G. & Battisti A. & **Taioli S.**

Microporous and Mesoporous Materials 143:46 (2011)

I am supervising or I supervised seven postdoctoral researchers:

- **Tommaso Morresi** at ECT\*, Trento on *Nucleosynthesis of heavy element in evo* from 01/07/2022 - to date

- **Achille Fiore** at ECT\*, Trento on *Microscopic calculations of nuclear structure and nucleosynthesis of heavy element during R process* from 01/04/2022 - to date

- **Paolo Emilio Trevisanutto** at ECT\*, Trento on *Artificial Intelligence for Quantum Systems* from 01/05/2019 - 31/08/2021

- **Samuel Giuliani** at ECT\*, Trento on *Microscopic calculations of nuclear structure and nucleosynthesis of heavy element during R process* from 01/12/2020 - 31/12/2021

- **Andrea Pedrielli** at ECT\* and at the Faculty of Mechanical Engineering, University of Trento on *Ab-initio simulation of the electronic, mechanical, and adsorption properties of materials* from 30/04/2018 - 31/09/2021

- **Pablo de Vera** Marie Curie Fellow at ECT\* on *Nanoparticle a Comprehensive Mechanistic description (NanoEnHanCeMent)* from 01/10/2020 - 31/09/2021

- **Alessio Paris** at at the European Centre for Theoretical Studies in Nuclear Physics and Related Areas from 01/01/2016 to 31/12/2017

Furthermore, I **supervised two master student dissertations:**

- Andrea Merlo (“Path integral Monte Carlo investigations of Li nucleosynthesis in evolved stars”)
- Stefano Nasca (“Graphene growth and functionalization: theory and calculations”)

## General scientific and academic activities

### Higher Assessment Committee Expert Council

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Member of the steering committee of the 2022 postdoctoral calls at ECT\*

### Editorial role

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**Associate Editor:** Frontiers in Materials – Editorial Board of the Computational Materials Science section

I am acting as **Topic Editor** for the research topic issue “Methodological and Computational Developments for Modeling the Transport of Particles within Materials” to appear in Frontiers in Materials. I acted as **Topic Editor** for the special issue “New Frontiers in Multiscale Modelling of Advanced Materials” appeared in Frontiers in Materials.

Also, I was **Guest Editor** for the 2014 Spring Meeting Proceedings of The Materials Research Society (MRS) and its publishing partner, Cambridge University Press.

### Reviewer’s experience

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I regularly **review** papers for several international high-impact journals in physics, chemistry and materials science, such as Physical Review Letters, Nature Communications, Science Advances, NanoLetters, Nanoscale, Communications Materials, Nanoscale Advances, ACS Materials and Interfaces, Industrial & Engineering Chemistry Research, Journal of Alloys and Compounds, Frontiers in Materials, Journal of Materials Chemistry A, Nuclear Instruments and Methods in Physics Research Section B, Frontiers in Materials, Reviews in Physics, Advances in Chemistry, Physical Review B, Scientific Reports, Physical Chemistry Chemical Physics, Chemical Science, The Journal of Physical Chemistry, The Journal of Physical Chemistry Letters, Physica E: Low-Dimensional Systems and Nanostructures, Physica B: Condensed Matter, Molecules, Journal of Molecular Modelling, Coordination Chemistry Reviews, Soft Computing, Journal of Hydrogen Energy, Journal of Physics B: Condensed Matter, Europhysics Letters, ....

### Recent Personal Research Grants and Project Funding

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**Mar 2022 – Feb 2026** : €2,896,705

*4D Microscopy of biological materials by short pulse terahertz sources (MIMOSA)*

**PRINCIPAL INVESTIGATOR** - granted by the European Community - PATHFINDER - OPEN

**Nov 2020 – Oct 2022** : €50,000

*Microscopic calculations of nuclear structure and nucleosynthesis of heavy element during R process*

**PRINCIPAL INVESTIGATOR** - granted by the Caritro Foundation



- Nov 2020 – Oct 2022** NanoEnHanCeMent: €171,473.28  
*Nanoparticle Enhanced Hadron-therapy: a Comprehensive Mechanistic description project*  
**CO-PRINCIPAL INVESTIGATOR (PI: Pablo de Vera)** H2020-MSCA-IF-2018 - granted by EU (contract n. 840752)
- Sept 2020 – Sept 2024** PANDORA: €3,500,000  
*Plasma for Astrophysics, Nuclear Decays Observation and Radiation for Archaeometry*  
**PROJECT LOCAL LEADER** - granted by INFN
- Nov 2020 – Oct 2023** QUICHE: €66,000  
*QUantum SensIng TeChnology for Fundamental PHysics Experiments*  
**CO-PRINCIPAL INVESTIGATOR** - granted by the Q@TN consortium
- Nov 2020 – Oct 2023** NADIA: €66,000  
*Quantum sensing with laser-synthesized nano-diamond NV color centers*  
**CO-PRINCIPAL INVESTIGATOR** - granted by the Q@TN consortium
- Nov 2019 – Oct 2022** ML Q-FORGE: €66,000  
*Machine Learning techniques FOR Quantum Gate Engineering*  
**CO-PRINCIPAL INVESTIGATOR** - granted by the Q@TN consortium
- Nov 2019 – Oct 2021** NANOCATER: €66,000  
*High-Z ceramic oxide nanosystems for mediated proton cancer therapy*  
**CO-PRINCIPAL INVESTIGATOR** - granted by the Caritro Foundation
- July 2018 – Aug 2021** ARTIQS: €240,000  
*ARTificial Intelligence for Quantum Systems*  
**CO-PRINCIPAL INVESTIGATOR** - granted by the Q@TN consortium
- Nov 2016 – Dec 2020** NEMESYS: €300,000  
*Non equilibrium dynamics models and excited state properties of low-dimensional systems*  
**CO-PRINCIPAL INVESTIGATOR** - granted by National Institute of Nuclear Physics (INFN)
- Mar 2013 – Oct 2016** MADELENA: €1,500,000  
*Developing and studying Novel Intelligent NanoMaterials and Devices towards Adaptive Electronics and Neuroscience Applications*  
**CO-PRINCIPAL INVESTIGATOR** - granted by Autonomous province of Trento on a competitive basis
- Dec 2010 – Dec 2015** The annual budget of the research group I led (2 post-docs, 4 staff and 3 PhD student) was around €500,000, based on both institutional support, public grants and industry income (almost 40 %).
- Mar 2014 – Aug 2014** : visiting scientist, Ecole Normale Supérieure de Lyon €8,000  
*Outgoing researcher grant: Bio-inspired electrochromic ink*  
**PRINCIPAL INVESTIGATOR** - granted by Autonomous province of Trento on a competitive basis
- Mar 2013 – Feb 2014** SuperCar: €30,000  
*Carbon-based nanomaterials and graphene growth on metallic substrates by supersonic fullerene epitaxy*  
**PRINCIPAL INVESTIGATOR** - granted by Autonomous province of Trento on a competitive basis
- Apr 2012 – July 2012** INTELBIOMAT visiting scientist, Pierre and Marie Curie University, Paris (FR): € 5,100  
*Interdisciplinary Approaches to Functional Electronic and Biological Materials*  
**PRINCIPAL INVESTIGATOR** - granted by the European Science Foundation

- Jan 2011 – Dec 2013** NATO Collaborative Linkage Grant: € 20,000  
Exchange Grants on electron energy loss techniques in collaboration with Kurchatov Institute, Moscow (RU)  
**CO-PRINCIPAL INVESTIGATOR** - granted by NATO
- Mar 2011 – Feb 2013** MISTICO: € 120,000  
*New Technologies and Microsystems for solar energy cogeneration solutions*  
**CO-PRINCIPAL INVESTIGATOR** - granted by the Caritro Foundation
- Jan 2010 – Dec 2010** *A comparative study of the electronic properties of graphene and hexagonal boron nitride monolayers on metal surfaces*  
Beam time at BESSY synchrotron radiation facility, Berlin (DE)  
**CO-PRINCIPAL INVESTIGATOR** - granted by BESSY consortium
- June 2010 – June 2011** Grant for computational time, 2,000,000 Au on Cray XT4: £ 3,000  
*A comparative study of the electronic properties of graphene and hexagonal boron nitride monolayers on metal surfaces*  
**PRINCIPAL INVESTIGATOR** - granted by EPSRC (UK)
- June 2010 – Dec 2010** Marie Curie Outgoing Researcher (FP7 People): € 30,000 *Epitaxial growth of graphene and SiC layers on inorganic surfaces: a joint theoretical and experimental approach.*  
**PRINCIPAL INVESTIGATOR** - granted by the European Commission
- Feb 2009 – Feb 2010** ETH consulting service agreement: € 54,000  
*Simulation and modeling of low energy electron beams*  
**CO-PRINCIPAL INVESTIGATOR** - granted by ETH, Zurich
- Feb 2007 – Dec 2007** Royal society International Joint Projects.  
*Melting curve of transition metals from first principles* £ 5,000  
**CO-PRINCIPAL INVESTIGATOR** - granted by the Royal Society
- Jan 2006** UCL Graduate School Award for Staff: £ 5,000  
*Wavepacket treatment of dissociative attachment of water*  
**PRINCIPAL INVESTIGATOR** - granted by University College London graduate school

## Visiting positions

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- Visiting professor - University of Murcia - 2 months (2021-2022)
- Visiting professor - Gdańsk University of Technology - 1 month (2021-2022)
- Research Fellow at the Institute of Advanced Studies - University of Bologna - 12 months (2012-2015)
- Visiting scientist - Ecole Normale Supérieure de Lyon - 6 months (2014)
- Visiting scientist - University Pierre and Marie Curie - 6 months (2013)
- Visiting scientist & Honorary Research Fellow - University College London - 10 months (2010)

## Invited talks

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- INVITED KEYNOTE and Session Chairman: **The Growth of Carbon-Based Materials by Supersonic Beam Epitaxy: Experiments, Theory and Calculations** – *Materials Research Society Meeting* – 21-24/04/2014, San Francisco (USA)

- INVITED speaker: **Theoretical Estimates of Stellar e-captures from First-Principles Simulations** – *Russbach School on Nuclear Astrophysics* – 08-14/03/2015, Russbach am Pass Gschütt, Austria
- INVITED speaker: **Electron-matter interaction as a tool for materials analysis: theory and experiment** – *Third joint CNR-FBK-UNITN Workshop* – 16/06/2015, University of Trento (IT)
- INVITED PLENARY lecture: *From materials science to astrophysics with multichannel scattering theory* – **Nanoscience & Nanotechnology 2015** – 28/09/2015-02/10/2015, INFN Frascati (Rome, IT)
- INVITED talk: **Graphene trumpets, foams, pillared networks, carbon materials growth, and all that from first-principles** – *EMN Meeting on Computation and Theory* – 10-14/10/2016, Las Vegas (USA)
- INVITED Talk: **Synthesis of carbon-based materials by SuMBE: theory and experiment** – *1st Synthetic methods across the flagship* – 6-10/02/2017, Puerto de la Cruz (Tenerife, SP)
- INVITED Talk: **A first-principle approach to scattering in many-body systems** – *14th International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2018)* – 14-18/03/2018, Thessaloniki (Greece)
- INVITED Talk: **The physics and chemistry of carbon** – *International Workshop on Nanocarbon Photonics and Optoelectronics (NPO2018)* – 6-10/08/2018, Savonlinna (FI)
- INVITED Talk: **Enabling materials by dimensionality: from 0D to 3D carbon-based nanostructures** – *15th International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2019)* – 01-05/05/2019, Rhodes (Greece)
- INVITED Talk: **Relativistic Theory and Ab Initio Simulations of Electroweak Decay Spectra in Medium-Heavy Nuclei** – *Precise beta decay calculations for searches for new physics* – 8-12/04/2019, ECT\*, Trento (Italy)
- INVITED Talk: **Relativistic Approaches to  $\beta$ -decays in stellar plasmas** – *PANDORA: Measuring  $\beta$ -decays in plasmas* – 30-31/10/2019, Perugia (Italy)
- INVITED Talk: **Exploring Event Horizons and Hawking Radiation through Deformed Graphene Membranes** – *Global Summit and Expo on Graphene and 2D Materials (2DMAT2021)* – 23-25/08/2021, Paris (France)
- INVITED PLENARY lecture: *17th International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2021)* – 04-07/09/2021, Heraklion, Crete (Greece)
- INVITED Talk and Session Chairman: **Simulation of low energy electron transport in condensed matter for technological and medical applications** – *Dynamics of Systems on the Nanoscale (DySoN-ISACC 2021)* – 18-22/10/2021, Santa Margherita Ligure (Italy)
- INVITED Talk: **The half-life for the radioactive  $^{134}\text{C}$ s and  $^{135}\text{C}$ s in astrophysical scenarios** – *2<sup>nd</sup> PANDORA Progress Meeting* – 16-17/12/2021, Catania (Italy)
- INVITED Talk: **Radioactive decay in evolved stars: the case of  $^{134}\text{C}$ s and  $^{135}\text{C}$ s** – *13th Torino Workshop on AGB stars & the 3rd Perugia Workshop on Nuclear Astrophysics* – 19-24/06/2022, Perugia (Italy)
- INVITED Talk: **Relative Role of Physical Mechanisms on Complex Biodamage Induced by Carbon Irradiation** – *From Hadrons to therapy: fundamental physics driving new medical advances* – 05-09/09/2022, Trento (Italy)

INVITED Talk: **Electronic excitation spectra and yield: from ab initio dielectric response functions to charge transport Monte Carlo simulations** – (*CMD30-FisMat2023*) – 04-08/09/2023, Milano

INVITED Talk: **From materials science to astrophysics with electronic structure simulations** – (*IOP-FHI workshop on the frontiers of electronic-structure theory and materials genomics*) – 16-19/10/2023, Beijing

INVITED SEMINARS: I delivered about 15 invited guest seminars at several chemistry, physics and materials engineering departments in Italy and Europe, including Charles University in Prague, EPFL in Lausanne, University of Trento, Ecole Normale Supérieure de Lyon, University of Bologna, University of Padua, University of Alicante, University of Murcia.

## Contributed talks

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Talk: **Exploring the wavepacket land: Dissociative Electron Attachment calculations** – *Winter School on Theoretical Methods for Electron and Positron Induced Chemistry* – 14-18/02/2005, J. Heyrovsky Institute of Physical Chemistry, Prague (CZ)

Talk: **Mixed ab initio quantum mechanical and Monte Carlo calculations of secondary emission from SiO<sub>2</sub> and carbon-based nanoclusters** – *Linking nuclei, molecules, and condensed matter: computational quantum many-body approaches* – 06-10/07/2009, ECT\*, Trento (IT)

Talk: **Scattering approach to the calculation of Auger spectra in nanostructures** – *13th European Conference on Applications of Surface and Interface Analysis* – 18-23/10/2009, Antalya, Turkey

Talk: **SURPRISES: when ab initio meets statistics in extended systems** – *International Workshop on Quantum Monte Carlo in the Apuan Alps VI* – 24-31/07/2010, The Apuan Alps Centre for Physics, Vallico Sotto (IT)

Talk: **Is contact potential the hallmark of the fermion-fermion interaction?** – *Sixteenth Training Course in the Physics of Strongly Correlated Systems* – 03-14/10/2011, International Institute for Advanced Scientific Studies, Vietri sul mare (IT)

Talk: **Non-adiabatic ab-initio molecular dynamics of Supersonic Beam epitaxy of Silicon Carbide at room temperature** – *9th European Conference of Computational Chemistry* – 01-05/09/2013, Sopron (HU)

Talk: **Non-adiabatic ab initio molecular dynamics of supersonic beam epitaxy of silicon carbide at room temperature** – *Italian National Conference on Condensed Matter Physics Including Optics, Photonics, Liquids, Soft Matter* – 09-13/09/2013, Milan (IT)

Talk: **The growth of carbon-based materials by supersonic beam epitaxy: experiments, theory and calculations** – *27th Indian-Summer School on Graphene – the Bridge between Low- and High-Energy Physics* – 14-18/09/2015, Prague (CZ)

Talk: *Theoretical estimates of stellar e-captures and beta-decay from first-principles simulations* – **28th Indian-Summer School on Ab Initio Methods in Nuclear Physics** – 29/08/2016-02/09/2016, Prague (CZ)

Talk: **Graphene trumpets, foams, pillared networks, carbon materials growth, and all that from first-principles** – *1st European Conference on Chemistry of Two-Dimensional Materials (Chem2DMat)* – 22-26/08/2017, Strasbourg (FR)

Talk: **Graphene synthesis, carbon foams, pillared graphene, pseudospheres and all that from first-principles, multiscale simulations and experiments** – *Recent Progress in Graphene and Two-dimensional Materials Research Conference (RPGR2017)* – 19-22/09/2017, Singapore

Talk: **Relative role of the physical mechanisms on complex biodamage induced by carbon irradiation** – (*CMD30-FisMat2023*) – 04-08/09/2023, Milano

## Professional Associations

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- Trento Institute for Fundamental Physics and Applications (National Institute for Nuclear Physics – INFN/TIFPA) - 2015
- National Research Council - 2021
- National Institute for Astrophysics - 2023
- Accademia Roveretana degli Agiati di Scienze, Lettere ed Arti - 2017
- Professional Order of the Engineers of the Italian Republic, Chartered Engineer - 2001

## Spoken Languages

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- Italian – Mother tongue
- English – Proficient
- French – Beginner
- Spanish – Beginner
- Hungarian – Beginner