ACADEMIC PORTFOLIO

Simone Taioli

Present Position

Senior Research Scientist

European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT*)
Strada delle Tabarelle, 286 – 38123 Trento, Italy

&

Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

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Basic Information

Personal Data

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

Education: degrees and diplomas

October 2009 – April 2013: 2^{nd} PhD in Physics (**Doctor Eropaeus**), 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 (Cambridge, UK), Co-advisors: Dr. Stefano Simonucci (Camerino, Italy), Dr. M. Dapor (Trento, Italy).

January 2001 – May 2004: 1^{st} PhD in Nuclear Science and Technology, University of Bologna, 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 (Camerino, Italy), Co-advisor: Prof. Renato Colle (Bologna, Italy)

October 1994 – December 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 (Bologna, Italy), Co-advisor: Dr. Stefano Simonucci (Camerino, Italy).

Previous employment

May 2010 – December 2014 Tenured position as Solid State and Materials Science **group leader** at the Interdisciplinary Laboratory for Computational Science, Center for Materials and Microsystems, Bruno Kessler Foundation, 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.

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

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

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

Previous occupation

August 2000 – July 2001 Military service.

Academic Habilitations to teach at Italian Universities

National Scientific Habilitation to Full Professor in **Theoretical Condensed Matter Physics**, Italy

National Scientific Habilitation to Associate Professor in **Theoretical Condensed Matter Physics**, Italy

National Scientific Habilitation to Associate Professor in **Models and Methods for the Chemical Sciences**, Italy

Qualification aux fonctions de maître de conférences **Milieux denses et matriaux**, France.

Research activity

Research Interests

- **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 computational 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.
- **Materials modelling under extreme conditions of temperature and pressure**, applied particularly to Earth and mineral sciences.
- **Modeling of carbon-based nanostructures**, such carbon nanotubes, fullerenes, graphene, graphene foams, functional materials or bio-inspired materials as well as memristive materials using a variety of *ab-initio*, atomistic and multiscale techniques for investigating ground and excited state electronic, optical, mechanical and thermodynamic properties.
- **Ultra-cold Fermi gases at unitarity** and BCS superconductivity.
- **Study from ab-initio and molecular mechanics simulations of hybrid organic-inorganic systems**, such as Metal-organic frameworks (MOF) and Zeolitic Imidazolate framework (ZIF), and organic, such as carbon foams and pillared graphene oxide for gas separation, storage and energy harvesting, also under high pressure.
- **Computational and experimental biophysics**: study of light-harvesting systems, such as multi-chromophoric Pigment Protein Complexes, bacteriochlorophyll, carotene, with both multi-reference methods typically used in quantum chemistry and experimental techniques, such as two-dimensional and pump-probe spectroscopy.
- **Development of novel methods to study β-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 equations, to interpret the β-decay spectra of heavy nuclei, such as lanthanides (used to develop scintillators for nuclear physics applications).
- **Computational modeling of crystal growth** from non-adiabatic molecular dynamics.
- **Monte Carlo modeling of the secondary electron emission** yield, of electron transport in solids, and of the response of solids to electromagnetic fields.
- **Physics of cancer and of its possible cure** (photodynamic therapy, proton-therapy) by computational modelling and experiments.

Conference organization

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)

Teaching and doctoral training

Course teaching: official responsibility

Course Teaching *Computational Materials Science*, a course for PhD students in Engineering at the University of Trento (2014–2015)
This included the preparation to produce teaching materials, final examinations and tutoring during the course

Course Teaching *Scattering theory with applications to Condensed Matter and Nuclear Physics*, 4^{th} and 5^{th} year physics student course, Charles University in Prague (Feb – June 2016)
This included the preparation to produce teaching materials, final examinations and tutoring during the course. Students' satisfaction and response was excellent

Advisory and co-advisory of master and postgraduate students

I am **supervising or supervised officially 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 Rèhault 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

Outcomes

1. **"Graphene trumpet black-hole analogue"**
   Morresi T. & Simonucci S. & Binosi D. & R. Piergallini & Roche S. & Pugno N. & **Taioli S.**
   Submitted to Nature Physics (June 2019)

2. **"Structural, Electronic and Mechanical properties of all-sp^2 graphene allotropes: the specific strength of tilene parent is higher than that of graphene and flakene has the minimal density"**
   Morresi T. & Pedrielli A. & Pugno N. & Gabbrielli R. & a Beccara S. & **Taioli S.**
   Submitted to 2D Materials (October 2018)

3. **"Anisotropic approach for simulating electron transport in layered materials: computational and experimental study of Highly Oriented Pyrolitic 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$_x$ 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) - **(https://onlinelibrary.wiley.com/doi/abs/10.1002/adts.201870030)**

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 **co-advised or am co-advising** 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

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.
   Submitted to Frontiers in Materials (July 2018)

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.
   Accepted in Journal of Physics: Condensed Matter (November 2018)

3. **"Anisotropic approach for simulating electron transport in layered materials: computational and experimental study of Highly Oriented Pyrolitic 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)

5. **"Energy deposition around carbon ion tracks in condensed water"**
   Azzolini M. & De Vera P. & Abril I & Garcia-Molina R. & Pugno N. & **Taioli S.** & Dapor M.
   To be submitted soon to J. Chem. Phys. C (November 2018)

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

Outcomes

1. **"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)

2. **"Gas Adsorption and Dynamics in Pillared Graphene Frameworks"**
   Pedrielli A. & **Taioli S.** & Garberoglio G. & Pugno N.
   Micropor. Mesopor. Mater. 257C, 222 (2018)

3. **"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)

4. **"A Novel Combined Experimental and Multiscale Theoretical Approach to Unravel the Structure of SiC/SiO_x 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_2, CH_4, N_2, and H_2 separation: a computer simulation investigation"**
   Garberoglio G. & Battisti A. & **Taioli S.**
   Microporous and Mesoporous Materials 143:46 (2011)

I am **supervising or supervised officially three postdoctoral students:**

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

Outcomes

1. **"Characterization of pristine and functionalized graphene on metal surfaces by electron spectroscopy"**
   Taioli S. & Paris A. & Calliari L.
   Handbook of Graphene, CRC Press, Chapter 18, 269-285 (2016)

2. **"Multiscale investigation of oxygen vacancies in TiO_2 anatase and their role in memristor's behavior"**
   Paris A. & **Taioli S.**
   J. Phys. Chem. C 120 (38), 22045 (2016)

- **Andrea Pedrielli** at the Faculty of Mechanical Engineering, University of Trento on *Simulation of the electronic, mechanical, and adsorption properties of materials* from 30/04/2018 todate

Outcomes

1. **"Structural, Electronic and Mechanical properties of all-sp^2 graphene allotropes: the specific strength of tilene parent is higher than that of graphene and flakene has the minimal density"**
   Morresi T. & Pedrielli A. & Pugno N. & Gabbrielli R. & a Beccara S. & **Taioli S.**
   Submitted to 2D Materials (October 2018)

- **A third post-doctoral position is to be assigned in January 2019** at the European Centre for Theoretical Studies in Nuclear Physics and Related Areas on *Artificial intelligence for Quantum Systems*

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")

Scientific activity

Editorial and reviewer's actvity

I regularly act as a **reviewer** for several international high-impact journals in physics, chemistry and materials science, such as Nature Communications, Science Advances, NanoLetters, 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, 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 etc.... Recently, I acted as **Topic Editor** for the volume "New Frontiers in Multiscale Modelling of Advanced

Materials" in Frontiers of 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. Furthermore, I delivered about 15 invited guest seminars at several chemistry, physics and materials engineering department in Italy and Europe, including Charles University in Prague, EPFL in Lausanne, University of Trento, Ecole Normale Superiore de Lyon, and University of Bologna.

Recent Personal Research Grants and Project Funding

July 2018 – August 2021 ARTIQS:€240.000
ARTificial Intelligence for Quantum Systems, granted by the Q@TN consortium

November 2016 – presently NEMESYS:€300.000
Non equilibrium dynamics models and excited state properties of low-dimensional systems, granted by National Institute of Nuclear Physics (INFN)

March 2013 – October 2016 MadElena: €1.500.000
"Developing and studying Novel Intelligent NanoMaterials and Devices towards Adaptive Electronics and Neuroscience Applications"

December 2010 – December 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 and grant income (almost 40 %). *Developing and Studying novel intelligent nanomaterials and Devices towards Adaptive Electronics and Neuroscience Applications*

March 2014 – August 2014 : visiting scientist, Ecole Normale Supérieure de Lyon €8.000
Outgoing researcher grant on "Bio-inspired electrochromic ink"

March 2013 – February 2014 SuperCar: €30.000
Carbon-based nanomaterials and graphene growth on metallic substrates by supersonic fullerene epitaxy

April 2012 – July 2012 INTELBIOMAT visiting scientist, Pierre and Marie Curie University, Paris (FR): € 5100.
Interdisciplinary Approaches to Functional Electronic and Biological Materials.

January 2011 – December 2013 NATO Collaborative Linkage Grant: € 20.000.
Exchange Grants on electron energy loss techniques in collaboration with Kurchatov Institute, Moscow (RU)

March 2011 – February 2013 Caritro Foundation: € 120.000.
Project **MISTICO***: New Technologies and Microsystems for solar energy cogeneration solutions*

January 2010 – presently Beam time at BESSY synchrotron radiation facility, Berlin (DE)
A comparative study of the electronic properties of graphene and hexagonal boron nitride monolayers on metal surfaces

June 2010 – June 2011 Grant for computational time, 2.000.000 Au on Cray XT4: £ 30,000.
A comparative study of the electronic properties of graphene and hexagonal boron nitride monolayers on metal surfaces

June 2010 – December 2010 Marie Curie Outgoing Researcher (FP7 People) to be spent at UCL: € 30.000.
Epitaxial growth of graphene and SiC layers on inorganic surfaces: a joint theoretical and experimental approach.

February 2009 – February 2010 ETH consulting service agreement: € 54.000.
Simulation and modeling of low energy electron beams.

February 2007 – December 2007 Royal society International Joint Projects.
Melting curve of transition metals from first principles, together with Prof. D. Alfè.

January 2006 UCL Graduate School Award for Staff: £ 5.000.
Wavepacket treatment of dissociative attachment of water.

Visiting positions and awards

Research Fellow at the Institute of Advanced Studies - University of Bologna - (2012-2015)

Visiting scientist - Ecole Normale Supérieure de Lyon - 6 months (2014)

Visiting scientist - University Pierre and Marie Curie - Paris VI - 6 months (2013)

Visiting scientist & Honorary Research Fellow - University College London (2010)

Talks

Invited talks

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 Gschútt, 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: **Nanoscience & Nanotechnology 2015** – *From materials science to astrophysics with multichannel scattering theory* – 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: **Black-hole carbon analogue** – *15th International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2019)* – 01-05/05/2019, Rhodos (Greece)

INVITED Talk: **Relativistic Theory and Ab Initio Simulations of Electroweak Decay Spectra in MediumHeavy Nuclei** – *Precise beta decay calculations for searches for new physics* – 8-12/04/2019, ECT*, Trento (Italy)

Contributed talks

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 SiO2 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 end 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

Professional Memberships and Affiliations

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

Spoken Languages

- Italian – Mother tongue
- English – Excellent both written and oral
- French – Basic
- Hungarian – Beginner

PUBLICATIONS

1) Enabling materials by dimensionality: from 0D to 3D carbon-based nanostructures
Simone Taioli
Accepted in "*Theoretical Chemistry for Advanced Nanomaterials - Functional Analysis by Computation and Experiment*", Springer-Berlin (February 2019)

2) The effects of a revised ^{7}Be e^{-}-capture rate on solar neutrino fluxes
Diego Vescovi, Luciano Piersanti, Sergio Cristallo, Maurizio Busso, Francesco Vissani, Sara Palmerini, Stefano Simonucci, **Simone Taioli**
Astronomy & Astrophysics A126, 7 (2019)

3) Production and processing of graphene and related materials
Claudia Backes, Amor M. Abdelkader, Concepción Alonso, Amandine Andrieux, Raul Arenal, Jon Azpeitia, Nilanthy Balakrishnan, Luca Banszerus, Julien Barjon, Ruben Bartali, Sebastiano Bellani, Claire Berger, Reinhard Berger, M.M. Bernal Ortega, Carlo Bernard, Peter H. Beton, André Beyer, Alberto Bianco, Peter Bøggild, Francesco Bonaccorso, Timoth J. Booth, Gabriela Borin Barin, Cristina Botas, Rebeca A. Bueno, Daniel Carriazo, Andres Catellanos-Gomez, Meganne Christian, Artur Ciesielski, Tymoteusz Ciuk, Matthew T. Cole, Jonathan Coleman, Camilla Coletti, Luigi Crema, Huanyao Cun, Daniela Dasler, D. De Fazio, Noel Díez, Simon Drieschner, Georg S. Duesberg, Roman Fasel, Xinliang Feng, Alberto Fina, Stiven Forti, Constantine Galiotis, Giovanni Garberoglio, Jorge M. García, Jose Antonio Garrido, Marco Gibertini, Armin Gölzhäuser, Julio Gómez, Thomas Greber, Frank Hauke, Adrian Hemmi, Iren Hernandez-Rodriguez, Andreas Hirsch, Stephen A. Hodge, Yves Huttel, Peter U. Jepsen, Ignacio Jimenez, Ute Kaiser, Tommi Kaplas, HoKwon Kim, Andras Kis, Papagelis Konstantinos, Kostas Kostarelos, Aleksandra Krajewska, Kangho Lee, Changfeng Li, Harri Lipsanen, Andrea Liscio, Martin R. Lohe, Annick Loiseau, Lucia Lombardi, Maria Francisca López, Oliver Martin, Cristina Martín, Lidia Martínez, Jose Angel Martin-Gago, Jose Ignacio Martinez, Nicola Marzari, Álvaro Mayoral, John McManus, Manuela Melucci, Javier Méndez, Cesar Merino, Pablo Merino, Andreas P. Meyer, Elisa Miniussi,Vaidotas Miseikis, Neeraj Mishra, Vittorio Morandi, Carmen Munuera, Roberto Muñoz, Hugo Nolan, Luca Ortolani, Anna K. Ott, Irene Palacio, Vincenzo Palermo, John, Parthenios, Iwona Pasternak, Amalia Patane, Maurizio Prato, Henri Prevost, Vladimir, Prudkovskiy, Nicola M Pugno, Teófilo Rojo, Antonio Rossi, Pascal Ruffieux, Paolo Samorì, Léonard Schué, Eki Setijadi, Thomas Seyller, Abhay Shivayogimath, Giorgio Speranza, Christoph Stampfer, Ingrid Stenger, Wlodek Strupinski, Yuri Svirko, **Simone Taioli**, Kenneth, B.K. Teo, Matteo Testi, Flavia Tomarchio, Mauro Tortello, Emanuele Treossi, Andrey Turchanin, Ester Vazquez, Elvira Villaro, Patrick R. Whelan, Zhenyuan Xia, RositzaYakimova, Sheng Yang, G. Reza Yazdi, Chanyoung Yim, Duhee Yoon, Xianghui Zhang, Xiaodong Zhuang, Luigi Colombo, Andrea C. Ferrari, Mar Garcia-Hernandez
Accepted in *2D Materials* (March 2019)

4) Secondary electron emission and yield spectra of metals from Monte Carlo simulations and experiments
Martina Azzolini, Marco Angelucci, Roberto Cimino, Rosanna Larciprete, Nicola M Pugno, **Simone Taioli**, Maurizio Dapor

Journal of Physics: Condensed Matter 31, 055901 (2019)

5) Ultrafast Carotenoid to Retinal Energy Transfer in Xanthorhodopsin Revealed by the Combination of Transient Absorption and Two−Dimensional Electronic Spectroscopy
Francesco Segatta, Itay Gdor, Julien Réhault, **Simone Taioli**, Noga Friedman, Mordechai Sheves, Ivan Rivalta, Sanford Ruhman, Giulio Cerullo, Marco Garavell
Chemistry–A European Journal 24 (46), 12084-12092 (2018)

6) Relativistic Theory and Ab Initio Simulations of Electroweak Decay Spectra in Medium-Heavy Nuclei and of Atomic and Molecular Electronic Structure
Tommaso Morresi, **Simone Taioli**, Stefano Simonucci
Advanced Theory and Simulations 1800086, 1-24 (2018)
JOURNAL COVER (https://onlinelibrary.wiley.com/doi/abs/10.1002/adts.201870030)

7) A novel combined experimental and multiscale theoretical approach to unravel the structure of SiC/SiOx core/shell nanowires for their optimal design
Tommaso Morresi, Melanie Timpel, Andrea Pedrielli, Giovanni Garberoglio, Roberta Tatti, Roberto Verucchi, Luca Pasquali, Nicola M Pugno, Marco Vittorio Nardi, **Simone Taioli**
Nanoscale 10, 13449-13461 (2018)

8) Anisotropic Approach for Simulating Electron Transport in Layered Materials: Computational and Experimental Study of Highly Oriented Pyrolitic Graphite
Martina Azzolini, Tommaso Morresi, Kerry Abrams, Robert Masters, Nicola Stehling, Cornelia Rodenburg, Nicola M Pugno, **Simone Taioli**, Maurizio Dapor
The Journal of Physical Chemistry C 122 (18), 10159-10166 (2018)

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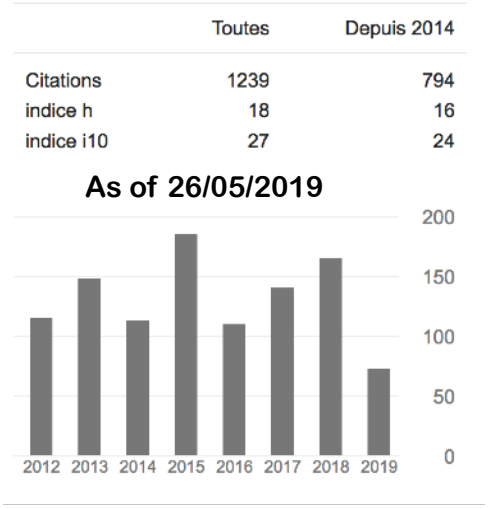

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