ACADEMIC PORTFOLIO

Simone Taioli

Personal Data

Date of birth:	27/09/1974
Place of birth:	Cesena (Italy)
Citizenship:	Italian
Gender:	Male
Office telephone:	+39 0461 314732
e-mail:	taioli@ectstar.eu
web:	https://www.ectstar.eu/people/detail/simone-taioli/
web:	https://en.wiki.topitalianscientists.org/Simone_Taioli

Current appointment

Senior Research Scientist

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

Education and previous academic appointments

Higher education

Oct 2009 – Apr 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 (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^{st} 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

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

August 2000 – July 2001 Compulsory military service.

Academic Habilitations to teach at Italian and European Universities

- 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

- **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 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 approximation, to interpret the β-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

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

- *Density functional approaches to the many-body problem*, 3^{rd} 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^{th} 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^{rd} 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^{th} and 5^{th} 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

I am currently **co-supervising two PhD students:**

- **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 **co-supervised two 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.

I **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 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. 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^2 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 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) - 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 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)

- **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_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 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

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

Editorial role

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

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

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

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 (last 10 years or so)

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 Talk: **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 Talk: **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, Rhodos (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 β-decays in stellar plasmas** – *PANDORA: Measuring β-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}Cs and ^{135}Cs in astrophysical scenarios** – *2^{nd} PANDORA Progress Meeting* – 16-17/12/2021, Catania (Italy)

INVITED Talk: **Radioactive decay in evolved stars: the case of ^{134}Cs and ^{135}Cs** – *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, Milan

INVITED Talk: **Electron collisions: From materials science to astrophysics** – *4th DEA Club Meeting* – 19-21/06/2024, Potsdam

INVITED Talk: **Towards realistic secondary electron simulation** – *FIT4NANO* – 27-28/06/2024, Vienna

INVITED Talk: **The influence of electronic correlation on weak decays of light and heavy nuclei in astrophysical scenarios** – *KRINA2025* – 17-21/02/2025, Trento (Italy)

INVITED Talk: **Advancements in secondary and backscattered electron energy spectra and yields analysis: From theory to applications** – *FisMat2025* – 07-11/09/2025, Venice

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, The Polytechnic University of Milan.

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)

INVITED Talk: **Adventures in the wavepacket land: DEA of water** – *International Symposium on Electron-Molecule Collisions and Swarms (EMS2005)* – 27-30/07/2005, Campinas (Brasil)

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

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

Talk: **Evaporation of cations from non-conductive nano-samples using single-cycle THz pulses: an experimental and theoretical study** – *International Symposium on Ultrafast Phenomena and THz Waves (ISUPTW)* – 15-18/11/2024, Guangzhou (China)

Talk: **Ab Initio Simulations of Electroweak Decay Spectra in astrophysical scenarios: the role of the electronic structure** – *s, i & r Element Nucleosynthesis (sirEN) Conference* – 08-13/06/2025, Giulianova

Professional Associations

- 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

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

PUBLICATIONS

1) Adsorption of Silica Oligomers on Biomolecules: Structural and Dynamical Insights for Atom Probe Tomography via classic Molecular Dynamics Simulations
Giovanni Novi Inverardi, Lorenzo Petrolli, Francesco Carnovale, **Simone Taioli**, Alessio Bartocci, Gianluca Lattanzi
Submitted to ***Computational and Structural Biotechnology Journal*** (2025)

2) Evaporation of cations from non-conductive nano-samples using single-cycle THz pulses: an experimental and theoretical study
M De Tullio, G Novi Inverardi, J Houard, M Ropitaux, I Blum, F Carnovale, Gianluca Lattanzi, **Simone Taioli**, G Eriksson, M Hulander, M Andersson, A Vella, T Morresi
Physical Review B 111 (4) (2025)

3) The role of primary and secondary electrons in scanning transmission electron microscopy of hybrid perovskites: the CsPbBr3 case
PE Trevisanutto, **Simone Taioli**, M Dapor, CS Allen, G Teobaldi
arXiv preprint arXiv:2412.16704 (2025)

4) Plasma Induced Variation of Electron Capture and Bound-State Decays
B Mishra, A Pidatella, **Simone Taioli**, S Simonucci, D Mascali
arXiv preprint arXiv:2407.01787 (2025)

5) Advancements in secondary and backscattered electron energy spectra and yields analysis: From theory to applications
Simone Taioli, M Dapor
Surface Science Reports 80, 100646 (2025)

6) Self-Locking in Collapsed Carbon Nanotube Stacks via Molecular Dynamics
A Pedrielli, **Simone Taioli**, NM Pugno
International Journal of Molecular Sciences 25 (19), 10635 (2024)

7) Atom probe tomography: Computational challenges and perspectives
G Lattanzi, **Simone Taioli**, GN Inverardi, F Carnovale
Biophysical Journal 123 (3), 424a (2024)

8) Nuclear physics midterm plan at LNS
C Agodi, F Cappuzzello, G Cardella, GAP Cirrone, E De Filippo, …, **Simone Taioli**, …
The European Physical Journal Plus 138 (11), 1038 (2023)

9) Editorial: Methodological and Computational Developments for Modeling the Transport of Particles within Materials
Maurizio Dapor, Rafael Garcia-Molina, Paolo Emilio Trevisanutto, Zejun Ding, **Simone Taioli**
Frontiers in Materials 10 (2023)

10) Silica In Silico: A Molecular Dynamics Characterization of the Early Stages of Protein Embedding for Atom Probe Tomography
Giovanni Novi Inverardi,Francesco Carnovale,Lorenzo Petrolli, **Simone Taioli,** Gianluca Lattanzi
Biophysica 3, 276 (2023)

11) A new approach to β-decays studies impacting nuclear physics and astrophysics: The PANDORA setup
David Mascali, Domenico Santonocito, Maurizio Busso, Luigi Celona, Alessio Galatà, Marco La Cognata, Giorgio Sebastiano. Mauro, Alberto Mengoni, Eugenia Naselli, Fabrizio Odorici, Sara Palmerini, Angelo Pidatella, Richard Ràcz, **Simone Taioli**, Giuseppe Torrisi
EPJ Web Conf. 279, 06006 (2023)

12) Presolar grain isotopic ratios as constraints to nuclear physics inputs for s-process calculations,
Sara Palmerini, Maurizio Busso, Diego Vescovi, Sergio Cristallo, Alberto Mengoni, Stefano Simonucci, **Simone Taioli**
EPJ Web Conf. 279 06007 (2023)

13) The role of low-energy electrons in the charging process of LISA test masses
Simone Taioli, Maurizio Dapor , Francesco Dimiccoli, Michele Fabi, Valerio Ferroni, Catia Grimani, Mattia Villani, William Joseph Weber
Classical and Quantum Gravity 40, 075001 (2023)

14) Elastic scattering of electrons by water: an ab initio study
Francesca Triggiani, Tommaso Morrresi, **Simone Taioli,** Stefano Simonucci
Frontiers in Materials 10, 1145261 (2023)

15) The role of molecular structure in Monte Carlo Simulations of the Secondary Electron Yield and Backscattering Coefficient from Methacrylic Acid
Katarzyna Wiciak-Pawłowska, Anna Winiarska**, Simone Taioli,** Maurizio Dapor, Małgorzata Franz, Jan Franz
Molecules 28(3), 1126 (2023)

16) Mechanical Properties of Twisted Carbon Nanotube Bundles with Carbon Linkers from Molecular Dynamics Simulations
Andrea Pedrielli, Maurizio Dapor, Konstantinos Gkagkas**, Simone Taioli,** Nicola Pugno
International Journal of Molecular Sciences 24(3), 2473 (2023)

17) Simulating the nanometric track-structure of carbon ion beams in liquid water at energies relevant for hadrontherapy
Pablo De Vera, Stefano Simonucci, Paolo Trevisanutto, Isabel Abril, Maurizio Dapor, **Simone Taioli**, Rafael Garcia-Molina,
J. Phys.: Conf. Ser. 2326, 012017 (2022)

18) A novel approach to β-decay: PANDORA, a new experimental setup for future in-plasma measurements
David Mascali, …., **Simone Taioli**, *et al.*
Universe 8, 80 (2022)

19) In search of the ground state crystal structure of Ta_2O_5 from ab-initio and Monte Carlo simulations
Andrea Pedrielli, Nicola Pugno, Maurizio Dapor, **Simone Taioli**
Computational Materials Science 216, 111828 (2022)

20) Energy Deposition around Swift Carbon-Ion Tracks in Liquid Water
Pablo De Vera, **Simone Taioli**, Paolo Trevisanutto, Isabel Abril, Rafael Garcia-Molina, Maurizio Dapor
International Journal of Molecular Sciences 23(11), 6121 (2022)

21) Theoretical estimate of the half-life for the radioactive ^{134}Cs and ^{135}Cs in astrophysical scenarios
Simone Taioli, Diego Vescovi, Sara Palmerini, Maurizio Busso, Sergio Cristallo, Alberto Mengoni, Stefano Simonucci
The Astrophysical Journal 933, 158 (2022)

22) Understanding Anharmonic Effects on Hydrogen Desorption Characteristics of Mg_nH_{2n} Nanoclusters by ab initio trained Deep Neural Network
Andrea Pedrielli, Paolo Emilio Trevisanutto, Lorenzo Monacelli, Giovanni Garberoglio, Nicola Pugno, **Simone Taioli**
Nanoscale, 14, 5589 (2022)

23) Presolar grain isotopic ratios as constraints to nuclear and stellar parameters of AGB nucleosynthesis
Sara Palmerini, Maurizio Busso, Diego Vescovi, Eugenia Naselli, Angelo Pidatella, Riccardo Mucciola, Sergio Cristallo, David Mascali, Alberto Mengoni, Stefano Simonucci, **Simone Taioli**
The Astrophysical Journal 921, 7 (2021)

24) Computational methods for 2D materials modelling
Alexandra Carvalho, Paolo Emilio Trevisanutto, **Simone Taioli**, Antonio Castro Neto
Reports on Progress in Physics 84, 106501 (2021)

25) Relativistic quantum theory and algorithms: a toolbox for modeling many-fermion systems in different scenarios
Simone Taioli, Stefano Simonucci
Annual Reports in Computational Chemistry **17** (2021)

26) Electronic excitation spectra of cerium oxides: from ab initio dielectric response functions to Monte Carlo electron transport simulations
Andrea Pedrielli, Pablo De Vera, Paolo Emilio Trevisanutto, Nicola Pugno, Isabel Abril, Rafael Garcia-Molina, **Simone Taioli**, Maurizio Dapor
Physical Chemistry Chemical Physics 23, 19173 (2021)
JOURNAL BACKCOVER (https://pubs.rsc.org/en/content/articlelanding/2021/cp/d1cp90186a)

27) The Resonant and Normal Auger spectra of ozone
Simone Taioli, Stefano Simonucci
Symmetry 13 (3), 516 (2021)

28) Relative role of the physical mechanisms on complex biodamage induced by carbon irradiation
Simone Taioli, Paolo Emilio Trevisanutto, Pablo De Vera, Isabel Abril, Rafael Garcia-Molina, Maurizio Dapor
The Journal of Chemical Physics Letters 12, 487 (2021)

29) Structural, Electronic and Mechanical properties of all-sp^2 graphene allotropes with density lower than graphene
Tommaso Morresi, Andrea Pedrielli, Ruggero Gabbrielli, Silvio a Beccara, Nicola Pugno, **Simone Taioli**
Carbon 159, 512 (2020)

30) Exploring Event Horizons and Hawking Radiation through Deformed Graphene Membranes
Tommaso Morresi, Daniele Binosi, Stefano Simonucci, Riccardo Piergallini, Stephan Roche, Nicola Pugno, **Simone Taioli**
2D Materials 7, 041006 (2020)
Covered by ***La Repubblica*** (https://www.repubblica.it/scienze/2020/07/14/news/)

31) Computational tools for calculating REEL spectra in solids: a comparison between Monte Carlo method and the numerical solution of the Ambartsumian-Chandrasekhar equations
Martina Azzolini, Olga Y. Ridzel, Pavel S. Kaplya, Viktor Afanas'ev, Nicola M Pugno, **Simone Taioli**, Maurizio Dapor
Computational Materials Science 173, 109420 (2020)

32) Production and processing of graphene and related materials
Claudia Backes, …, **Simone Taioli**, *et al.*
2D Materials 7 (2), 022001 (2020)

33) Enabling materials by dimensionality: from 0D to 3D carbon-based nanostructures
Simone Taioli
In "***Theoretical Chemistry for Advanced Nanomaterials - Functional Analysis by Computation and Experiment***", Springer-Berlin (March 2020)

34) VizieR Online Data Catalog: Effects of a revised 7Be e-capture rate
Diego Vescovi, Luciano Piersanti, Sergio Cristallo, Maurizio Busso, Francesco Vissani, Sara Palmerini, Stefano Simonucci, **Simone Taioli**
VizieR Online Data Catalog 362 (2019)

35) 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)

36) 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)

37) 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)

38) 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)

39) 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)

40) 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)

41) UV-light induced vibrational coherences, the key to understand Kasha rule violation in trans-azobenzene
Artur Nenov, Rocio Borrego-Varillas, Aurelio Oriana, Lucia Ganzer, Francesco Segatta, Irene Conti, Javier Segarra-Martí, Junko Omachi, Maurizio Dapor, **Simone Taioli**, Cristian Manzoni, Shaul Mukamel, Giulio Cerullo, Marco Garavelli
The journal of physical chemistry letters 9, 1534-1541 6 (2018)

42) Gas adsorption and dynamics in Pillared Graphene Frameworks
Andrea Pedrielli, **Simone Taioli**, Giovanni Garberoglio, Nicola M Pugno
Microporous and Mesoporous Materials 257, 222-231 (2018)

43) Mechanical and thermal properties of Graphene Random nanofoams via Molecular Dynamics simulations
Andrea Pedrielli, **Simone Taioli**, Giovanni Garberoglio, Nicola M Pugno
Carbon 132, 766-775 (2018)

44) 2D Material Armors Showing Superior Impact Strength of Few Layers
Stefano Signetti, **Simone Taioli**, Nicola M Pugno
ACS Applied Materials & Interfaces 9 (46), 40820–40830 (2017)

45) Spider silk reinforced by graphene or carbon nanotubes
Emiliano Lepore, Federico Bosia, Francesco Bonaccorso, Matteo Bruna, **Simone Taioli**, Giovanni Garberoglio, Andrea Ferrari, Nicola Pugno
2D Materials 4 (3), 031013 (2017)
Covered by The EU GRAPHENE FLAGSHIP (https://cordis.europa.eu/article/id/122640-where-nature-meets-science-spider-webs-made-out-of-graphene)

46) Monte Carlo simulations of measured electron energy-loss spectra of diamond and graphite: role of dielectric-response models
Martina Azzolini, Tommaso Morresi, Giovanni Garberoglio, Lucia Calliari, Nicola M Pugno, **Simone Taioli**, Maurizio Dapor
Carbon 118, 299 (2017)

47) A quantum chemical interpretation of two-dimensional electronic spectroscopy of Light-Harvesting complexes
Francesco Segatta, Lorenzo Cupellini, Sandro Jurinovich, Shaul Mukamel, Maurizio Dapor, Simone Taioli, Marco Garavelli, Benedetta Mennucci
Journal of the American Chemical Society 139 (22), 7558 (2017)

48) Designing graphene based nanofoams with nonlinear auxetic and anisotropic mechanical properties under tension or compression
Andrea Pedrielli, **Simone Taioli**, Giovanni Garberoglio, Nicola M Pugno
Carbon 111, 796-806 (2017)

49) Multiscale Investigation of Oxygen Vacancies in TiO2 Anatase and Their Role in Memristor's Behavior
Alessio Paris, **Simone Taioli**
The Journal of Physical Chemistry C 120 (38), 22045–22053 (2016)

50) Characterization of Pristine and Functionalized Graphene on Metal Surfaces by Electron Spectroscopy
Simone Taioli, Alessio Paris, Lucia Calliari
Graphene Science Handbook: Size-Dependent Properties 5, 269–285 (2016)

51) Lobachevsky crystallography made real through carbon pseudospheres
Simone Taioli, Ruggero Gabbrielli, Stefano Simonucci, Nicola M Pugno, Alfredo Iorio
Journal of Physics: Condensed Matter 28 (13), 13LT01 (2016)

52) A bird's eye view on the concept of multichannel scattering with applications to materials science, condensed matter, and nuclear astrophysics
Simone Taioli
Frontiers in Materials, 30 (2016)

53) Synthesis of single layer graphene on Cu (111) by C 60 supersonic molecular beam epitaxy
Roberta Tatti, Lucrezia Aversa, Roberto Verucchi, Emanuele Cavaliere, Giovanni Garberoglio, Nicola M Pugno, Giorgio Speranza, **Simone Taioli**
RSC Advances 6 (44), 37982-37993 (2016)

54) Lithium abundances in AGB stars and a new estimate for the 7Be life-time
Sara Palmerini, Maurizio Busso, Stefano Simonucci, **Simone Taioli**
Journal of Physics: Conference Series 665 (1), 012014 (2016)

55) New Frontiers in Multiscale Modelling of Advanced Materials
Simone Taioli, Maurizio Dapor, Nicola Pugno
Frontiers in Materials 2, 71 (2015)

56) The interaction of C60 on Si(111) 7 × 7 studied by supersonic molecular beams: interplay between precursor kinetic energy and substrate temperature in surface activated processes
Lucrezia Aversa, **Simone Taioli**, Marco Nardi, Roberta Tatti, Roberto Verucchi, Salvatore Iannotta
Frontiers in Materials 2, 46 (2015)

57) A computational perspective on multichannel scattering theory with applications to physical and nuclear chemistry
Simone Taioli, Stefano Simonucci
Annual Reports in Computational Chemistry 11, 191-310 (2015)

58) Tetrapeptide unfolding dynamics followed by core-level spectroscopy: a first-principles approach
Simone Taioli, Stefano Simonucci, Silvio a Beccara, Marco Garavelli
Physical Chemistry Chemical Physics 17, 11269-11276 (2015)

59) Gas Adsorption and Separation in Realistic and Idealized Frameworks of Organic Pillared Graphene: A Comparative Study
Giovanni Garberoglio, Nicola Pugno, **Simone Taioli**
The Journal of Physical Chemistry C 119, 1980-1987 (2014)

60) Computational study of graphene growth on copper by first-principles and kinetic Monte Carlo calculations
Simone Taioli
Journal of molecular modeling 20 (7), 2260 (2014)

61) The BEC-BCS crossover in ultracold Fermi gases beyond the contact-potential approximation
Giovanni Garberoglio, **Simone Taioli**, Stefano Simonucci
The European Physical Journal D 67 (6), 129 (2013)

62) Modeling the Li abundances of RGB and AGB stars with a new estimate for the 7 Be half-life
Maurizio Busso, Sara Palmerini, Stefano Simonucci, **Simone Taioli**, Sergio Cristallo, Carlos Abia, Stefan Uttenthaler
XII International Symposium on Nuclei in the Cosmos 146, 145 (2013)

63) From materials science to astrophysics with electronic structure calculations
Simone Taioli
http://eprints-phd.biblio.unitn.it/952/ University of Trento (2013)

64) Theoretical estimates of Stellar e–Captures. I. The half-life of 7Be in evolved stars
Stefano Simonucci, **Simone Taioli**, Sara Palmerini, Maurizio Busso
The Astrophysical Journal 764 (2), 118 (2013)

65) Non-adiabatic *ab initio* molecular dynamics of supersonic beam epitaxy of silicon carbide at room temperature
Simone Taioli, Giovanni Garberoglio, Stefano Simonucci, Silvio a Beccara, Lucrezia Aversa, Marco Nardi, Roberto Verucchi, Salvatore Iannotta, Maurizio Dapor, Dario Alfè
The Journal of chemical physics 138 (4), 044701 (2013)
JOURNAL COVER (https://aip.scitation.org/toc/jcp/138/4?expanded=138)

66) Nanotensile tests, microscopy characterization and atomistic simulations of carbon nanotubes fibers
Maria Pantano, Shanov Vesselin, Mark Schulz, Fedrizzi Michele, Iacob Erica, Bersani Massimo, **Simone Taioli**, Silvio a Beccara, Nicola M Pugno
NanotechItaly (2013)

67) An experimental/ab-initio study on carbon nanotubes fibers for application in high-performing sporting goods.
Maria F Pantano, Shanov Vesselin, Mark J Schulz, Michele Fedrizzi, Erica Iacob, Massimo Bersani, **Simone Taioli**, Silvio A Beccara, Nicola Pugno
The Winter Universiade Conference (2013)

68) Modeling flexibility in metal–organic frameworks: comparison between density-functional tight-binding and universal force field approaches for bonded interactions
Giovanni Garberoglio, **Simone Taioli**
Microporous and Mesoporous Materials 163, 215-220 (2012)

69) Epitaxy of nanocrystalline silicon carbide on Si (111) at room temperature
Roberto Verucchi, Lucrezia Aversa, Marco V Nardi, **Simone Taioli**, Silvio a Beccara, Dario Alfè, Lucia Nasi, Francesca Rossi, Giancarlo Salviati, Salvatore Iannotta
Journal of the American Chemical Society 134 (42), 17400-17403 (2012)

70) A scattering view of the Bogoliubov-de Gennes equations
Stefano Simonucci, Giovanni Garberoglio, **Simone Taioli**
AIP Conference Proceedings 1485 (1), 312-318 (2012)

71) Infrared spectroscopy of copper-resveratrol complexes: A joint experimental and theoretical study
Barbara Chiavarino, Maria E Crestoni, Simonetta Fornarini, **Simone Taioli**, Ines Mancini, Paolo Tosi
The Journal of chemical physics 137 (2), 024307 (2012)

72) Communication: electronic band gaps of semiconducting zig-zag carbon nanotubes from many-body perturbation theory calculations
Paolo Umari, Oleg Petrenko, **Simone Taioli**, Merlyne M De Souza
The Journal of chemical physics 136 (18), 181101 (2012)

73) Finite-range effects in dilute Fermi gases at unitarity
Stefano Simonucci, Giovanni Garberoglio, **Simone Taioli**
Physical Review A 84 (4), 043639 (2011)

74) Zeolitic imidazolate frameworks for separation of binary mixtures of CO2, CH4, N2 and H2: A computer simulation investigation
Anna Battisti, **Simone Taioli**, Giovanni Garberoglio
Microporous and Mesoporous Materials 143 (1), 46-53 (2011)

75) Direct observation of a dispersionless impurity band in hydrogenated graphene
Danny Haberer, Luca Petaccia, Mani Farjam, **Simone Taioli**, Seyed Jafari, Alexei Nefedov, W Zhang, Lucia Calliari, Giorgina Scarduelli, Balázs Dóra, Denis Vyalikh, Thomas Pichler, Christof Wöll, Dario Alfè, Stefano Simonucci, Mildred Dresselhaus, Martin Knupfer, Bernd Büchner, Alexander Grüneis
Physical Review B 83 (16), 165433 (2011)

76) Tunable band gap in hydrogenated quasi-free-standing graphene
Danny Haberer, Denis Vyalikh, **Simone Taioli**, Balázs Dóra, Mani Farjam, John Fink, Dmitry Marchenko, Thomas Pichler, Klaus Ziegler, Stefano Simonucci, Mildred Dresselhaus, Martin Knupfer, Bernd Buchner, Alexander Gruneis
Nano letters 10 (9), 3360-3366 (2010)

77) Electron spectroscopies and inelastic processes in nanoclusters and solids: theory and experiment
Simone Taioli, Stefano Simonucci, Lucia Calliari, Maurizio Dapor
Physics Reports 493 (5), 237-319 (2010)

78) Electronic properties of extended graphene nanomaterials from *GW* calculations
Simone Taioli, Paolo Umari, Merlyne De Souza
Physica status solidi (b) 246 (11-12), 2572-2576 (2009)

79) SURPRISES: when ab initio meets statistics in extended systems
Simone Taioli, Stefano Simonucci, Maurizio Dapor
Computational Science & Discovery 2 (1), 015002 (2009)

80) Mixed ab initio quantum mechanical and Monte Carlo calculations of secondary emission from SiO 2 nanoclusters
Simone Taioli, Stefano Simonucci, Lucia Calliari, Massimiliano Filippi, Maurizio Dapor
Physical Review B 79 (8), 085432 (2009)

81) Ab-initio melting curve and principal Hugoniot of tantalum
Simone Taioli, Claudio Cazorla, Mike Gillan, Dario Alfè
Journal of Physics: Conference Series 121 (1), 012010 (2008)

82) Melting curve and Hugoniot of molybdenum up to 400 GPa by ab initio simulations
Claudio Cazorla, Mike Gillan, **Simone Taioli**, D Alfè
Journal of Physics: Conference Series 121 (1), 012009 (2008)

83) Melting curve of tantalum from first principles
Simone Taioli, Claudio Cazorla, Mike Gillan, Dario Alfè
Physical Review B 75 (21), 214103 (2007)

84) *Ab initio* melting curve of molybdenum by the phase coexistence method
Claudio Cazorla, Mike Gillan, **Simone Taioli**, Dario Alfè
The Journal of chemical physics 126 (19), 194502 (2007)

85) A wave packet method for treating nuclear dynamics on complex potentials
Simone Taioli, Jonathan Tennyson
Journal of Physics B: Atomic, Molecular and Optical Physics 39 (21), 4379 (2006)

86) WATERWAVES: wave particles dynamics on a complex triatomic potential
Simone Taioli, Jonathan Tennyson
Computer physics communications 175 (1), 41-51 (2006)

87) Electron-molecule collisions at low and intermediate energies using the R-matrix method
Jimena Gorfinkiel, Alex Faure, **Simone Taioli**, Chiara Piccarreta, Gabriela Halmova, Jonathan Tennyson
The European Physical Journal D-Atomic, Molecular, Optical and Plasma (2005)

88) Auger-electron angular distributions calculated without the two-step approximation: Calculation of angle-resolved resonant Auger spectra of C 2 H 2
Renato Colle, Davide Embriaco, Micol Massini, Stefano Simonucci, **Simone Taioli**
Physical Review A 70 (4), 042708 (2004)

89) Ab initio calculation of the normal Auger spectrum of C2H2
Renato Colle, Davide Embriaco, Micol Massini, Stefano Simonucci, **Simone Taioli**
Journal of Physics B: Atomic, Molecular and Optical Physics 37 (6), 1237 (2004)

90) Atomic and molecular collisions and interactions-Auger-electron angular distributions calculated without the two-step approximation: Calculation of angle-resolved resonant Auger spectra of C2H2
Renato Colle, Davide Embriaco, Micol Massini, Stefano Simonucci, **Simone Taioli**
Physical Review-Section A-Atomic Molecular and Optical Physics 70 (4), 42708 (2004)

91) Ab initio calculation of the C1s photoelectron spectrum of C2H2
Renato Colle, Davide Embriaco, Micol Massini, Stefano Simonucci, **Simone Taioli**
Nuclear Instruments and Methods in Physics Research Section B (2004)

92) On the angular dependence of L x-ray production cross sections following photoionization at an energy of 59.54 keV
Agostino Tartari, Claudio Baraldi, Ernesto Casnati, Andrea Da Re, Jorge Fernandez, **Simone Taioli**
Journal of Physics B: Atomic, Molecular and Optical Physics 36 (5), 843 (2003)

OUTREACH JOURNALS

93) Eye, brain and color
Simone Taioli
Atti Acc. Rov. Agiati, a. 266, 2016, ser. IX, vol. VI, B: 35-64
(http://www.agiati.it/ara_context.jsp?ID_LINK=114269&area=196)

94) Bio-inspired materials. Lessons we can learn from Nature
Simone Taioli
Atti Acc. Rov. Agiati, a. 267, 2017, ser. IX, vol. VII, B: 71-89
(http://www.agiati.it/ara_context.jsp?ID_LINK=114572&area=196)