Curriculum Vitæ

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

Office telephone: +39 0461-314732
e-mail1: taioli@ectstar.eu

Personal Data

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

Research Interests

1. Development and application of state-of-the-art many-body techniques, from mean-field (Hartree-Fock and Density Functional Theory) to methods beyond mean-field, such as configuration interaction (CI), many-body perturbation theory (GW), and Path-Integral Monte Carlo (PIMC).

2. Development and application of scattering methods to study resonance-affected photo-excitation events in materials at different scales of aggregation in their interaction with external fields. I am one (among three) developer and maintainer of the SURPRISES code, a mixed *ab-initio* and Monte Carlo code suite to simulate electron spectra (XPS, Auger, ARPES, EELS, NEXAFS) of organic and inorganic molecules in gas or solid phase.

3. Development of novel methods to study β-decay in stellar nucleosynthesis of evolved stars and 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).

4. Materials modeling, particularly 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.

5. Ultra-cold Fermi gases at unitarity and BCS superconductivity.

6. Monte Carlo modeling of the secondary electron emission yield in dielectric materials (using time-dependent density functional theory).

7. Computational modeling of crystal growth, such as silicon carbide and graphene via supersonic molecular beam epitaxy.

8. Metal-organic frameworks and pillared graphene oxide for gas separation, storage and energy harvesting.

9. Study of the excited states in light-harvesting systems, such as multi-chromophoric Pigment Protein Complexes, bacteriochlorophyll, carotene, with multi-reference methods typically used in quantum chemistry.

Academic Habilitation

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

National Scientific Habilitation to Associate Professor in **Models and Methods for Chemical Sciences**.

Education

October 2009 – April 2013: PhD in Physics (**Doctor Eropaeus**), University of Trento, Trento (IT).

- Gained a second PhD in theoretical condensed matter physics. Final mark: **excellent.**
- Thesis title: "*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: PhD in Nuclear Science and Technology, University of Bologna, Bologna (IT) and Scuola Normale Superiore, Pisa (IT)

- **By competition scoring first.**
- Thesis title: "*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**).
- Thesis title: "*Quantum mechanical calculation of Auger spectra of silicon clusters.*".
- Advisor: Prof. Renato Colle (Bologna, Italy), Co-advisor: Dr. Stefano Simonucci (Camerino, Italy).

Academic positions

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 occupations

August 2000 – July 2001 Military service.

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)

Recent Personal Research Grants and Project Funding

November 2016 – presently NEMESYS:€300.000
it 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

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.

Teaching Activity

Course Teaching *Computational Materials Science*, a course for PhD students in Engineering at the University of Trento (2014–2015)

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)

Course Teaching *De novo density functional methods for ground and excited states*, a course for PhD students in Physics at the University of Trento (2017–2018)

Talks at conferences

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)

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)

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)

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)

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)

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)

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

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)

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)

The physics of black-hole analogues – European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT*) – Trento (IT)

Scientific activity

I regularly act as a reviewer for many 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, 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.
Finally, I act officially as a supervisor to 2 PhD students:
- Francesco Segatta at the Chemistry Department, University of Bologna on *Computational Based Design of Bio-Inspired Electrochromic Molecules for Colour Tunable Electronic Ink* from 01/10/2014
- Tommaso Morresi at Faculty of Mechanical Engineering, University of Trento on *Numerical simulations on the mechanics of nanocomposites based on graphene or other 2D materials* from 01/11/2015
With other two graduate students I am actively collaborating in the capacity of second supervisor.

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

Other activities

I played football at professional level, I am keen on jogging, climbing and practicing open-air sports. I am fond of Italian literature, poetry, and economics. In my spare time, I actively work in the voluntary sector.

Publications

1. **"On the angular dependence of L x-ray production cross sections following photoionization at an energy of 59.54 keV"**
   Tartari A. & Baraldi C.& Casnati E. & Da Re A. & Fernandez J. & **Taioli S.**
   J. Phys. B: Atom. Molec. Phys. 36:843 (2003)
2. **"Ab–initio calculation of the C1s photoelectron spectrum of C2H2"**
   Colle R. & Embriaco D. & Massini M. & Simonucci S. & **Taioli S.**
   Nuc. Inst. Meth. Phys. Res. B 213:65 (2003)
3. **"Ab–initio calculation of the normal Auger spectrum of C_2H_2"**
   Colle R. & Embriaco D. & Massini M.& Simonucci S. & **Taioli S.**
   J. Phys. B: Atom. Molec. Phys. 37:1237 (2004)
4. **"Auger-electron angular distributions calculated without the two-step approximation: Calculation of angle-resolved resonant Auger spectra of C_2H_2"**
   Colle R. & Embriaco D. & Massini M. & Simonucci S. & **Taioli S.**
   Phys. Rev. A 70:042708 (2004)
5. **"Inner shell photoionization and non-radiative decay processes in molecules: theory and calculations"**
   Taioli S.
   PhD Thesis: University of Bologna arXiv (2004)
6. **"Electron–molecules collisions at low and intermediate energies using the R-matrix method"**
   Gorfinkiel J. & Faure A. & **Taioli S.** & Piccarreta C. & Halmova G. & Tennyson J.
   Eur. Phys. J. At. Mol. Opt 35:231 (2005)
7. **"Wave particles dynamics on a complex triatomic potential"**
   Taioli S. & Tennyson J.
   Comp. Phys. Comm. 175:41 (2006)

8. **"WATERWAVES: Code suite"**
Taioli S. & Tennyson J.
Comp. Phys. Comm. Progr. Library, Catalogue identifier: ADXT_v1_0 (2006)
[http://cpc.cs.qub.ac.uk/cpc/]

9. **"A wave packet method for treating nuclear dynamics on complex potentials"**
Taioli S. & Tennyson J.
J. Phys. B: Atom. Molec. Phys. 39:4379 (2006)

10. **"Ab–initio Melting Curve of Molybdenum by the Phase Coexistence Method"**
Cazorla C. & **Taioli S.** & Alfè D. & Gillan M.J.
J. Chem. Phys. 126:194502 (2007)

11. **"Melting curve of Tantalum from first principles"**
Taioli S. & Cazorla C. & Gillan M.J. & Alfè D.
Phys. Rev. B 75:214103 (2007)

12. **"Ab-initio melting curve and principal Hugoniot of tantalum"**
Taioli S. & Cazorla C. & Gillan M.J. & Alfè D.
J. Phys. C: Cond. Mat. 121:012010 (2008)

13. **" Melting curve and Hugoniot of molybdenum up to 400 GPa by ab-initio simulations"**
Cazorla C. & **Taioli S.** & Alfè D. & Gillan M.J.
J. Phys. C: Cond. Mat. 102:012009 (2008)

14. **"Mixed ab initio quantum mechanical and Monte Carlo calculations of secondary emission from Si02 nanoclusters"**
Taioli S. & Simonucci S. & Calliari L.& Filippi M. & Dapor M.
Phys. Rev. B: Cond. Mat. 79:085432. (2009)

15. **"SURPRISES: When ab-initio meets statistics in extended systems"**
Taioli S. & Simonucci S. & Dapor M.
Comp. Sci. Disc. 2:015002 (2009)

16. **"Electronic properties of carbon based nanostructures from GW calculations"**
Taioli S. & Umari P. & De Souza M.M.
Phys. Stat. Sol. 246:1 (2009)

17. **"Tunable bandgap in hydrogenated quasi-free-standing graphene"**
Haberer D. & Vyalikh D.V. & **Taioli S.** & Dora B. & Farjam M. & Fink J. & Marchenko D. & Pichler T. & Ziegler K. & Simonucci S. & Dresselhaus M. S. & Knupfer M. & Büchner B. & Grüeneis A.
NanoLett. 10:3360 (2010)

18. **"Electron spectroscopies and inelastic processes in nanoclusters and solids: theory and experiment"**
Taioli S. & Simonucci S. & Calliari L. & Dapor M.
Phys. Rep. 493:237 (2010)

19. **"Zeolitic Imidazolate Frameworks for CO2/CH4 and CO2/H2 separation: a computer simulation investigation"**
Garberoglio G. & Battisti A. & **Taioli S.**
Microporous and Mesoporous Materials 143:46 (2011)

20. **"Direct observation of a dispersionless impurity band in hydrogenated graphene"**
Haberer D. & Petaccia L. & Farjam M. & **Taioli S.** & Jafari S. A.& Nefedov A. & Zhang W. & Calliari L. & Scarduelli G. & Dora B. & Vyalikh D.V. & Pichler T. & Woll Ch. & Alfè D. &

Simonucci S. & Dresselhaus M. S. & Knupfer M. & Buchner B. & A. Grüneis A.
Phys. Rev. B 83:165433 (2011)

21. **"Finite-range effects in dilute Fermi gases at unitarity"**
Simonucci S. & Garberoglio G. & **Taioli S.**
Phys. Rev. A 84:043639 (2011)

22. **"Electronic band gaps of semiconductor zig-zag carbon nanotubes from GW calculations"**
Umari P. &Petrenko O. & **Taioli S.** & De Souza M.M.
J. Chem. Phys. Comm. 136:181101 (2012) - Most downloaded paper May 2012

23. **"Infrared spectroscopy of copper-resveratrol complexes: a joint experimental and theoretical study"**
Chiavarino B. & Crestoni M.E. & Fornarini S. & **Taioli S.** & Mancini I. &Tosi P.
J. Chem. Phys. 137:024307 (2012)

24. **"A scattering view of the Bogoliubov-de Gennes equations"**
Simonucci S. & G. Garberoglio & **Taioli S.**
AIP Conf. Proc. 1485:312 (2012)

25. **"Modeling flexibility in Metal-Organic Frameworks: comparison between Density-Functional Tight-Binding and Universal Force Field approaches for bonded interactions "**
Garberoglio G. & **Taioli S.**
Micropor. Mesopor. Mater. 163:215 (2012)

26. **"Modeling the Li abundances of RGB and AGB stars with a new estimate for the ^{7}Be half-life time "**
Palmerini S.& Busso M. & Simonucci S. & **Taioli S.** & Cristallo S. & Abia C. & Uttenthaler S
Proceedings of Science - PoS(NIC XII)145

27. **"Epitaxy of nanocrystalline Silicon Carbide on Si(111) at room temperature"**
Verucchi R. & Aversa L. & Nardi M.V. & **Taioli S.** & a Beccara S. & Alfè D. & Nasi L. & Rossi F. & Salviati G. & Iannotta S.
J. Am. Chem. Soc. - Communications, 134:17400 (2012)

28. **"Theoretical Estimates of Stellar e$^-$ Captures. I. The half-life of ^{7}Be in Evolved Stars"**
Simonucci S. & **Taioli S.** & Palmerini S. & Busso M.
The Astrophysical Journal 764:118 (2013)

29. **"Non-adiabatic *ab-initio* molecular dynamics of Supersonic Beam epitaxy of Silicon Carbide at room temperature"**
Taioli S. & Garberoglio G. & Simonucci S. & a Beccara S. & Aversa L. & Nardi M.V. & Verucchi R. & Iannotta S & Alfè D.
J. Chem. Phys. 138:044701 (2013) - chosen as **JOURNAL COVER** in Volume 138 Issue 4 on 28 Jan. 2013

30. **"From materials science to astrophysics with electronic structure calculations"**
Taioli S.
http://eprints-phd.biblio.unitn.it/952/ (2013)

31. **"Solution of the Bogoliubov–de Gennes equations using multichannel scattering methods"**
Garberoglio G. & Simonucci S. & **Taioli S.**
European Physical Journal D 67:129 (2013)

32. **"Computational study of graphene growth on copper by first-principles and kinetic Monte Carlo calculation"**
Taioli S.
Journal of Molecular Modelling 20:2260 (2014)

33. **"Gas adsorption and separation in realistic and idealized frameworks of organic pillared graphene: a comparative study"**
Garberoglio G. & Pugno N. & **Taioli S.**
J. Phys. Chem. C 119:980 (2015)

34. **"Tetrapeptide unfolding dynamics followed by core-level spectroscopy: a first-principles approach."**
Taioli S. & Simonucci S.& a Beccara S. & Garavelli M.
Phys. Chem. Chem. Phys. 17:11269 (2015)

35. **"The interaction of C_{60} on Si(111) 7×7 studied by Supersonic Molecular Beams: interplay between precursor kinetic energy and substrate temperature in surface activated processes."**
Aversa L. & **Taioli S.** & Nardi M.V. & Tatti R. & Verucchi R. & Iannotta S.
Frontiers in Materials 2:46 (2015)

36. **"A computational perspective on multichannel scattering theory with applications to physical and nuclear chemistry"**
Taioli S.. & Simonucci S.
Annual Reports in Computational Chemistry Volume 11 (2015)

37. **"New Frontiers in Multiscale Modelling of Advanced Materials"**
Taioli S.. & Dapor M. & Pugno N.
Editorial - Frontiers in Materials 2:71 (2015)

38. **"Synthesis of single layer graphene on Cu (111) by C 60 supersonic molecular beam epitaxy"**
Tatti R. & Aversa L. & Verucchi R. & Cavaliere E. & Garberoglio G. & Pugno N & Speranza G. & **Taioli S.**
RSC Advances 6 (44), 37982 (2016)

39. **"Lobachevsky crystallography made real through carbon pseudospheres"**
Taioli S. & Gabbrielli R. & Simonucci S. & Pugno N. & Iorio A.
Journal of Physics: Condensed Matter 28 (13), 13LT01 (2016)

40. **"Lithium abundances in AGB stars and a new estimate for the ^{7}Be life-time"**
Palmerini S. & Busso M. & Simonucci S. & **Taioli S.**
Journal of Physics: Conference Series 665 (1), 012014 (2016)

41. **"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)

42. **"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)

43. **"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)

44. **"Monte Carlo simulations of measured electron energy-loss spectra of diamond and graphite: Role of dielectric-response models"**
M. Azzolini & T. Morresi & G. Garberoglio & L. Calliari & N. Pugno & **Taioli S.** & M. Dapor.
Carbon 118, 299 (2017)

45. **"A quantum chemical interpretation of 2DES spectra of Light-Harvesting complexes"**
F. Segatta & L. Cupellini & S. Jurinovich & S. Mukamel & M. Dapor & **Taioli S.** & M. Garavelli & B. Mennucci
J. Am. Chem. Soc. 139 (22), 7558 (2017)

46. **"Silk reinforced with graphene or carbon nanotubes spun by spiders"**
Lepore E. & Bonnaccorso F. & Bruna M. & Bosia F. & **Taioli S.** & Garberoglio G & Ferrari A.C. & Pugno N.
2D Materials, 4 (3), 031013 (2017)

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

48. **"White Book on Synthetic Methods"**
Taioli S. & Garberoglio G & Pugno N.
Accepted in 2D Materials (July 2017)

49. **"Design of graphene– and boron-nitride–based 2D multilayer nanoarmours"**
Taioli S. & Signetti S. & Pugno N.
Submitted to ACS Applied Materials & Interfaces (Aug. 2017)

50. **"Theory of β-decay in lanthanides"**
Morresi T. & **Taioli S.**. & Saltarelli & F. Camera & Simonucci S.
In preparation and to be submitted to Phys. Lett. B (Oct. 2017)

51. **"Estimates of Stellar e^- captures from first-principles and Path Integral Monte Carlo: a comparative study"**
Merlo A. &**Taioli S.** & Simonucci S. & Pederiva F.
In preparation and to be submitted to The Astrophysical Journal (Nov. 2017)

52. **"Electron-phonon driven Superconductivity in K_3C_{60} from first-principles calculations"**
Taioli S. & Casula M. & Calandra M & Mauri F.
In preparation (Jan. 2018)