

Europass Curriculum Vitae



Personal information

Surname(s) / First name(s)

Email(s)

Nationality(-ies)

Gender

Giacomazzi Luigi

lgiacomazzi@ung.si

Italiana

Male

Work experience

Dates

Occupation or position held

Name and address of employer

Dates

Occupation or position held

Name and address of employer

Dates

Occupation or position held

Name and address of employer

Dates

Occupation or position held

From 1 February 2022

Staff Researcher

• Research activity mainly concerning materials relevant for microelectronics and for the optical fibers technology (e.g. silicon, silica and other amorphous oxides). Study of point defects in these materials by means of first-principles techniques.

CNR-IOM/Democritos, c/o SISSA via Bonomea 265, 34136 Trieste (Italia).

From 1 October 2018 to January 2022

Assistant Professor

• Research activity concerning materials relevant for microelectronics and for the optical fibers technology e.g. silica and amorphous oxides such as NaPO_3 and P_2O_5 glasses. Study of point defects in pure and doped silica by means of first-principles techniques.

• Linear Algebra lecturer; Continuum Mechanics lecturer.

University of Nova Gorica, Materials research laboratory Vipavska 11c SI-5270 Ajdovscina (Slovenia)

From 1 April 2017 to 30 September 2018

Postdoc Talents³ fellowship (Assegno di ricerca).

• Within the recently obtained Talents3 fellowship (<https://www.areasciencepark.it/innovazione/programma-di-mobilita-internazionale-talents/>) investigations have carried out to study defects in rare-earth and rare-earth P-codoped silica based optical fibers. Given its relevance for the RE doping, also P-doped silica and P_2O_5 optical and vibrational properties have been studied (Outgoing phase started in April 2017 at the Materials Research Laboratory of the University of Nova Gorica, while return phase started in April 2018 at SISSA).

• Awarded with a computational grant through the HPC Challenge of Arctur d.o.o. (2018).

• ISCRA-B project leader. CINECA grant OXYRIS-HP10B5K2GU (2017).

Area Science park FVG Trieste (Italia)

From 1 September 2012 to 28 February 2017

Postdoc (Assegno di ricerca).

<p>Name and address of employer</p>	<ul style="list-style-type: none"> • Research project dedicated to color centers in pure, Ge-doped vitreous silica ($v\text{-SiO}_2$) and vitreous germania ($v\text{-GeO}_2$), the understanding of which is of paramount importance for improving the performances of silica-based optical fibers as well as microelectronic devices. This is especially true for applications in harsh-environments where a high concentration of these radiation-induced defects can stop the normal functioning of silica-based devices. In particular, a class of paramagnetic color centers in silica based materials, i.e. the E' centers, will be investigated by means of first-principles calculations of electron paramagnetic resonance (EPR) parameters by using the Quantum-Espresso package. • IS CRA-B project leader. CINECA grant OMEGAFIB-HP10BMKWVL (2015-2016). • IS CRA-B project leader. CINECA grant EPRFIBER-HP10B4CVBH (2013-2014). <p>CNR-IOM/Democritos, c/o SISSA via Bonomea 265, 34136 Trieste (Italia).</p>
<p>Dates</p>	<p>From 9 January 2012 to 30 June 2012.</p>
<p>Occupation or position held</p>	<p>Visiting scientist (Postdoc).</p>
<p>Main activities and responsibilities</p>	<ul style="list-style-type: none"> • Development of programs and scripts for calculating the dissociation constant of water at high pressure and temperature by using an ab-initio parametrized force field for water. • Research project "First-principles study of electronic defects in vitreous silica". This project especially aims at improving our understanding of silica under irradiation, e.g in optical fibers used in harsh-environments as in nuclear power plants (work in collaboration with Prof. S. Scandolo ICTP, Dr. L. Martin-Samos, University of Nova-Gorica, and Prof. S. De Gironcoli SISSA)
<p>Name and address of employer</p>	<p>The Abdus Salam International Centre for Theoretical Physics (ICTP).</p>
<p>Dates</p>	<p>From 16 December 2009 to 15 December 2011.</p>
<p>Occupation or position held</p>	<p>Postdoc.</p>
<p>Main activities and responsibilities</p>	<ul style="list-style-type: none"> • Testing and developing tasks for the GWL code for GW calculations of large systems such as organic dyes on a titania surface (work in collaboration with Dr. P. Umari, Università di Padova and Prof. F. De Angelis, Università di Perugia). Study of electronic, structural and vibrational properties of amorphous materials ($a\text{-Si}_3\text{N}_4$, $v\text{-GeSe}_2$, $v\text{-SiO}_2$). • Referee for an international founding agency and for international peer-review journals. • Use of the large computer facilities provided by CINECA (https://hpc.cineca.it/). • Maintenance of the package "Vibtools" for post-processing of vibrational spectra (www.qeforge.org).
<p>Name and address of employer</p>	<p>Scuola Internazionale Superiore di Studi Avanzati (SISSA), via Bonomea 265, 34126, Trieste (Italia).</p>
<p>Dates</p>	<p>From 15 March 2007 to 15 December 2009</p>
<p>Occupation or position held</p>	<p>Postdoc (Assegno di ricerca).</p>
<p>Main activities and responsibilities</p>	<ul style="list-style-type: none"> • Study of dislocation properties in coesite (SiO_2), and of high-pressure phase transitions of gypsum relevant for the understanding of Earth mantle rheology. Study of electronic, structural and vibrational properties of amorphous materials ($a\text{-Si}_3\text{N}_4$, $v\text{-GeO}_2$, $v\text{-SiO}_2$). • Referee for international peer-review journals (J. of Applied Physics; Physical Review B; J. of Physics-Condensed Matter) • Visit to LSPES laboratory (Lille, France) for scientific collaboration in the framework of the Postdoc research project concerning the study of dislocations in coesite. January 2009. • Visit to Kyoto University (Japan) for scientific collaboration in the framework of the Postdoc research project concerning the study of dislocations in coesite. March 2008.
<p>Name and address of employer</p>	<p>CNR-INFN/Democritos, Strada costiera 11, 34151 Trieste (Italia), at the Abdus Salam International Centre for Theoretical Physics (ICTP).</p>

Teaching experiences

- (From January 2019) Lecturer of the "Linear Algebra" course for physics and astronomy.
- (From 2020) Lecturer of the "Continuum Mechanics" course for physics and astronomy.
- (Feb–March 2012) Online tutor via MOODLE interface for the "Advanced Electromagnetism" course held at ICTP. Main tasks: write html documentation for the course lessons; provide students with materials (books, exercises, multiple choice quizzes, online lessons).
- (July 2010). Oral presentation: *Introduction to the VibTOOLS package*. CECAM tutorial: Simulating Spectroscopy using Quantum-ESPRESSO related codes. SISSA (Trieste, IT).

Mentoring experiences

- (From 2003 to 2006) I assisted Prof. A. Pasquarello for the lectures: *Cours de Physique générale III et IV pour Systèmes de Communication (3ème et 4ème semestres)*. In particular, I was involved in preparing exams and helping students to solve exercises classes.

- Supervising a "diploma seminar" project (UNG): *Vibrational spectra of am-Al₂O₃: tuning a parametric model*, J. Kurtović (February-August 2021).
- *Co-advisor of a diploma thesis project* of a student at ICTP (Mr. R. Kanak, Supervisor Prof. S. Scandolo): "the dissociation constant of water at extreme conditions: a molecular dynamics study" (April-June 2012).
- In 2010 I helped Prof. S. Baroni in supervising a first year SISSA PhD student (Xiaochuan Ge), whose project concerned the study of the absorption spectra of a class of natural dyes by using time dependent density functional techniques (Report 15/12/2010, "Seeing Colors With TDDFT").

Other academic achievements, honors, and activities

- French qualification aux fonctions de Maître de Conférences (2010).
- Chairman of the session "Defects and Modeling II" at The 12th International Symposium on SiO₂: SiO2018, (Bari, Italy) 11-13 June 2018.
- Individual membership of the Italian Physical Society (SIF).

Education and training

Dates	From 01/01/2003 to 04/03/2007.
Title of qualification awarded	Docteur ès Sciences.
Title of the Thesis	First principles vibrational spectra of tetrahedrally-bonded glasses: SiO ₂ , GeO ₂ , and GeSe ₂ .
Principal subjects/Occupational skills covered	<ul style="list-style-type: none">• Physics of glasses.• Programming in Fortran90, Bash, Perl, Python.• Preparing scientific papers (cfr. p. 3) and oral presentations concerning the PhD research project.• Use of the large computer facilities provided by CSCS (www.cscs.ch) e dell'EPFL.• Use of the programs in the Quantum ESPRESSO package for electronic structure calculations. Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland.
Name and type of organization providing education and training	
Dates	2002
Title of qualification awarded	Degree in Physics with marks 110/110 <i>cum laude</i>
Title of the Thesis	Proprietà dinamiche di ⁴ He liquido: risultati della Teoria del Funzionale Densità.
Principal subjects/Occupational skills covered	<ul style="list-style-type: none">• State solid physics.• Programming in Fortran90, C++, Matlab.• Writing of scientific manuscripts by using \LaTeX. Università degli Studi di Padova, Italia
Name and type of organization providing education and training	
Dates	1997
Title of qualification awarded	Diploma di Maturità scientifica with marks 57/60
Name and type of organization providing education and training	Liceo scientifico "Tito Lucrezio Caro", Cittadella, Padova.

Personal skills and competences

Mother tongue(s)

Other language(s)

Self-assessment
European level^(*)

English

French

Slovenian

German

Italiano

Understanding				Speaking				Writing	
Listening		Reading		Spoken interaction		Spoken production			
C1	Proficient user	C1	Proficient user	C1	Proficient user	B2	Independent user	C1	Proficient user
B2	Independent user	C1	Proficient user	C1	Proficient user	B2	Independent user	B2	Independent user
A2	Basic user	A2	Basic user	A2	Basic user	A2	Basic user	A2	Basic user
A1	Basic user	A1	Basic user	A1	Basic user	A1	Basic user	A1	Basic user

^(*) Common European Framework of Reference (CEF) level

Computational Packages

- Quantum Espresso; Lammps; CP2K

Computer skills and competences

- Experience with Linux e Unix operative systems.
- Good knowledge of \LaTeX , obtained by self-teaching and from professional context.
- Good knowledge of the programming language Fortran90, obtained by self-teaching and from professional context.
- General knowledge of the programming languages C++, Bash, Perl, Matlab, Python, obtained by self-teaching (Matlab), professional context (Bash, Python) and introductory courses (C++ e Perl).
- General knowledge of the packages Office e OpenOffice, obtained by self-teaching.

Driving licence(s)

Italian "Patente B" (European driving licence).

Additional information

Marital status

Married with children

Selection of attended lectures and courses

Slovene language course, UNG, Nova Gorica, 2019.

School on Electron-Phonon Physics from First Principles (free listener). ICTP Trieste (IT), March 2018.

Basic Slovene language course. SISSA Club, SISSA Trieste (IT), Feb–June 2014.

Basic course on how to use the IBM Sp6 platform. ICTP, Trieste (IT), Nov. 2009.

Programming course: Perl. EPFL, Lausanne (CH), October 2006.

Parallel programming course: *Parallel programming workshop: an introduction into the basics of parallel programming*. CSCS, Lugano (CH), August 2005.

Corso di *Tecniche di debugging e di ottimizzazione di codici scalari e paralleli*. CINECA, Bologna (IT), October 2004.

Cours de français B2. Centre de langue de l'EPFL, Lausanne (CH), March–June 2004.

Corso sul *calcolo delle proprietà elettroniche, strutturali e dinamiche dei materiali: un'introduzione pratica all'uso del package PWscf-FPMD-CP*. CINECA, Bologna (IT), March 2004.

Cours de français B1. Centre de langue de l'EPFL, Lausanne (CH), March–June 2003.

Basic German language course. Centro Diffusione Lingue, Padova (IT), July 2002.

C++ programming course. Mathematics Department of the University of Padova. March–May 2002.

Selected Publications (h-index 15, citations 714, source Researchgate 19/10/2022)

- 1 I. Reghioua, L. Giacomazzi *et al.* "O₂ Loaded Germanosilicate Optical Fibers: Experimental In Situ Investigation and Ab Initio Simulation Study of GLPC Evolution under Irradiation", *Applied Sciences* **12**, 3916 (2022)
- 2 L. Giacomazzi *et al.* "Paramagnetic Intrinsic Point Defects in Alkali Phosphate Glasses: Unravelling the P3 Center Origin and Local Environment Effects," *J. Physical Chemistry C* **125**, 8741 (2021).
- 3 N. Salles, L. Martin-Samos, S. de Gironcoli, L. Giacomazzi, M. Valant, A. Hemeryck, P. Blaise, B. Sklenard, N. Richard, "Collective dipole effects in Ionic Transport under electric fields", *Nature Commun.* **11**, 3330 (2020).
- 4 N.S. Shcheblanov, L. Giacomazzi, M.E. Povarnitsyn, S. Kohara *et al.*, "Vibrational and structural properties of glass: Advances from a combined modeling approach", *Phys. Rev. B* **100**, 134309 (2019).
- 5 L. Giacomazzi *et al.* "v-P2O5 micro-clustering in P-doped silica studied by a first-principles Raman investigation", *Sci. Reports* **9**, 7126 (2019).
- 6 D. A. J. Whittaker, L. Giacomazzi, Devashibhai Adroja, S. M. Bennington, A. Pasquarello, and P. S. Salmon, "Partial vibrational density of states for amorphous solids from inelastic neutron scattering," *Phys. Rev. B* **98**, 064205 (2018).
- 7 L. Giacomazzi, L. Martin-Samos, A. Alessi, M. Valant, K.C. Gunturu, A. Boukenter, Y. Ouerdane, S. Girard, N. Richard, "Optical absorption spectra of P defects in vitreous silica", *Opt. Mater. Express* **8**, 385 (2018).
- 8 L. Giacomazzi, L. Martin-Samos, A. Alessi, A. Boukenter, Y. Ouerdane, S. Girard, S. De Gironcoli, and N. Richard, "Photoactivated processes in optical fibers: generation and conversion mechanisms of twofold coordinated Si and Ge atoms.", *Nanotechnology* **28**, 195202 (2017).
- 9 B. Winkler, L. Martin-Samos, N. Richard, L. Giacomazzi, A. Alessi, S. Girard, A. Boukenter, Y. Ouerdane, and M. Valant, "Correlations Between Structural and Optical Properties of Peroxy Bridges from First-Principles." *J. Phys. Chem. C* **121**, 402 (2017).
- 10 S. Girard, A. Boukenter, Y. Ouerdane, N. Richard, C. Marcandella, P. Paillet, L. Martin-Samos, and L. Giacomazzi, "Radiation Effects on Optical Fibers and Fiber-Based Sensors, in *Ionizing Radiation Effects in Electronics: From Memories to Imagers*", ed. M. Bagatin, S. Gerardin, CRC Press (2015).
- 11 L. Giacomazzi, L. Martin-Samos, N. Richard, "Paramagnetic centers in amorphous GeO₂", *Microelectron. Eng.* **147**, 130 (2015).
- 12 L. Giacomazzi, L. Martin-Samos, A. Boukenter, Y. Ouerdane, S. Girard, and N. Richard, "Ge(2), Ge(1) and Ge-E' centers in irradiated Ge-doped silica: a first-principles EPR study", *Opt. Mater. Express* **5**, 1054 (2015).
- 13 L. Giacomazzi, L. Martin-Samos, A. Boukenter, Y. Ouerdane, S. Girard, N. Richard "EPR parameters of E' centers in v-SiO₂ from first-principles calculations", *Phys. Rev. B* **90**, 014108 (2014).
- 14 P. Umari, L. Giacomazzi, F. De Angelis, M. Pastore, and S. Baroni, "Energy-level alignment in organic dye-sensitized TiO₂ from GW calculations.", *Journal of Chemical Physics* **139**, 014709 (2013).
- 15 Luigi Giacomazzi, C. Massobrio, and A. Pasquarello, "Vibrational properties of vitreous GeSe₂ with BLYP density functional." *Journal of Physics-Condensed Matter* **23**, 295401 (2011).
- 16 P. Umari, X. Qian, N. Marzari, G. Stenuit, L. Giacomazzi, and S. Baroni, "Accelerating GW calculations with optimal polarizability basis." *Physica Status Solidi B* **248**, 527 (2011).
- 17 L. Giacomazzi, P. Carrez, S. Scandolo, and P. Cordier, "Dislocation properties of coesite from an ab-initio parametrized interatomic potential." *Physical Review B* **83**, 014110 (2011).
- 18 Luigi Giacomazzi and S. Scandolo, "Gypsum under pressure: a first-principles study." *Physical Review B* **81**, 064103 (2010).
- 19 Luigi Giacomazzi and P. Umari, "First-principles investigation of electronic, structural and vibrational properties of a-Si₃N₄." *Physical Review B* **80**, 144201 (2009).
- 20 Luigi Giacomazzi, P. Umari, and A. Pasquarello, "Medium-range structure of vitreous SiO₂ obtained through first-principles investigation of vibrational spectra." *Physical Review B* **79**, 064202 (2009).
- 21 Luigi Giacomazzi and A. Pasquarello, "Vibrational spectra of vitreous SiO₂ and vitreous GeO₂ from first principles." *Journal of Physics-Condensed Matter* **19**, 415112 (2007).
- 22 Luigi Giacomazzi, C. Massobrio, and A. Pasquarello, "First-principles investigation of the structural and vibrational properties of vitreous GeSe₂." *Physical Review B* **75**, 174207 (2007).
- 23 Luigi Giacomazzi, P. Umari, and A. Pasquarello, "Vibrational spectra of vitreous germania from first-principles." *Physical Review B* **74**, 155208 (2006).

- 24 Luigi Giacomazzi, P. Umari, and A. Pasquarello, "Medium-Range Structural Properties of Vitreous Germania Obtained through First-Principles Analysis of Vibrational Spectra." *Physical Review Letters*, **95**, 075505 (2005).
- 25 Luigi Giacomazzi, F. Toigo, and F. Ancilotto, "Dynamics of liquid ^4He in confined geometries from time-dependent density functional calculations." *Physical Review B* **67**, 104501 (2003).

Selected Conferences and Talks.

- 0 Oral presentation: *Unravelling the P_3 centers origin in alkali phosphate glasses*, 27th Annual meeting of the Slovenian Chemical Society, 22-24 Sept. 2021, Portoroz.
- 1 Oral contribution: *Unravelling the P_3 centers origin in alkali phosphate glasses*, 107th Congresso nazionale Società Italiana di Fisica (SIF) 13-17 Sept. 2021 (Online).
- 1 Oral presentation: *$v\text{-}P_2O_5$ "micro-clusters" in P-doped silica studied by a first-principles Raman investigation*. 25th Annual meeting of the Slovenian Chemical Society, 25-27 Sept. 2019, Maribor.
- 2 Oral presentation (invited): *Color centers in P-doped silica: generation, conversion mechanisms and optical properties*. The 12th International Symposium on SiO₂: SiO2018, (Bari, Italy) 11-13 June 2018.
- 3 Oral presentation: *Color centers in P-doped silica optical fibers: a first-principles investigation*. 8^{mes} Journées sur les Fibres Optiques en Milieu Radiatif, University of Mons, (Mons, Belgium) 11-12 Dec. 2017.
- 4 Oral presentation: *Color centers in P-doped and Yb-doped silica optical fibers: a first-principles investigation*. FisMat2017, (Trieste, Italy), 1-5 Oct. 2017.
- 5 Oral presentation: *Paramagnetic H-related defects in silica: a first-principles investigation*., CMMSE2016 (Cadiz, Spain) July 4-8, 2016.
- 6 Oral presentation: *Spectroscopie théorique (RPE, Raman, ...): état de l'art+exemples+limitations*, Workshop Approche Couplée, University of Saint-Etienne, June 16-17, 2016.
- 7 Poster presentation: *First-principles calculations of EPR parameters of P-related defects in SiO₂*, 11th International Symposium on SiO₂, University of Nice (Nice, France), 13 Jun–15 June 2016.
- 8 Oral presentation: *First-principles investigation of paramagnetic centers in $v\text{-SiO}_2$, Ge-doped SiO₂ and $v\text{-GeO}_2$* . FisMat2015, (Palermo, Italy), 27 Sept. - 2. Oct. 2015.
- 9 Poster presentation: *Paramagnetic centers in $\alpha\text{-GeO}_2$* . INFOS2015, University of Udine (Udine, Italy), 29 Jun–2 July 2015.
- 10 Poster presentation: *Unravelling the origin of the E'_α and Ge(2) centers*. *Total Energy, ICTP(Trieste, Italy)*. 15–17 Jan. 2015
- 11 Oral presentation: *First-principles calculations of EPR parameters of E' centers in $v\text{-SiO}_2$* . Eurodim2014 (Canterbury, United Kingdom). 13–19 July 2014.
- 12 Oral presentation: *First-principles calculations of EPR parameters of vacancy-related defects in $v\text{-SiO}_2$* .. SiO₂ 2014 Symposium (Cagliari, Italy). 16–18 June 2014.
- 13 Oral presentation: *Radiation induced color centers in Silica: a first-principles investigation*.. CMSE2013 (Almeria, Spain). 24–27 June 2013.
- 14 Participation to 3^{mes} Journées sur les Fibres Optiques en Milieu Radiatif, University of Nice, (Nice, France) 12-13 nov. 2012.
- 15 Oral presentation: *First-principles investigation of chemical disorder in Vitreous GeSe₂*. ESG2012 (Maastricht, Hollande). 3–6 June 2012.
- 16 Poster presentation: *First-principles study of electronic defects in silica glass*. ESG2012 (Maastricht, Hollande). 3–6 June 2012.
- 17 Poster presentation: *Many Body Perturbation Theory simulations of the electronic properties of large systems*. CECAM workshop: Challenges and Solutions in GW Calculations for Complex Systems UNIL (Lausanne, Switzerland). 7–10 June 2011.
- 18 Poster presentation: *First-Principles Investigation of $\alpha\text{-Si}_3\text{N}_4$* . CECAM workshop: Which Electronic Structure Method for the Study of Defects? EPFL (Lausanne, Switzerland). June 2009.
- 19 Oral presentation: *Vibrational spectra of vitreous SiO₂ and vitreous GeO₂ from first-principles*. CECAM workshop: Mineral spectroscopy by theory and experiment. EPFL (Lausanne, Switzerland). Oct. 2008.
- 20 Posters presentation: *Generalized stacking fault energy surfaces and dislocations properties in Coesite and First-Principles Investigation of the Structural and Vibrational Properties of $\alpha\text{-Si}_3\text{N}_4$* . CPMD workshop. ICTP (Trieste, IT). June 2008.

- 21 | Oral presentation (Invited): *Vibrational spectra of vitreous SiO₂ and vitreous GeO₂ from first-principles*. CECAM workshop: Glasses meet Glasses (Lyon, France). June 2007.
- 22 | Poster presentation: *Vibrational spectra of vitreous GeO₂ and vitreous GeSe₂ from first-principles*. First EuroMinSci Conference (La Colle sur Loup, Nice, France). March 2007.
- 23 | Oral presentation: *Medium-Range Structural Properties of Vitreous Germania Obtained through First-Principles Analysis of Vibrational Spectra*. APS March Meeting (Baltimore, USA). March 2006.