Silvia Mauri | Curriculum Vitae

Date and place of birth:
Civil status:

EDUCATION AND TRAINING

University of Trieste - CNR IOM **Trieste, Italy**
PhD in Nanotechnology (Settore scientifico disciplinare FIS/03) *November 1st, 2019 - May 22th, 2023*

Laboratory: APE-HE beamline, Elettra Synchrotron (Trieste). The PhD thesis has been submitted on January 31th 2023, and it has been evaluated positively by two referees (grade: excellent), no further revision was needed. The scientific research carried out during the PhD is part of the NFFA Trieste project (https://www.trieste.nffa.eu/).

- Supervisor: Dr. Piero Torelli

- Thesis title: "Operando Soft X-Ray Absorption Spectroscopy Applications for the Investigation of Surface Reactivity of Heterogeneous Catalysts for Methanol Valorization".
  The PhD project aimed to improve and exploit the potentialities of a homemade apparatus able to perform ambient pressure *operando* NEXAFS experiments on the APE-HE beamline at Elettra Synchrotron. In detail, the reaction cell has been used to study the surface reactivity of heterogeneous catalysts of different compositions, combining the NEXAFS spectroscopy with complementary techniques such as DRIFTS, SEM, theoretical DFT calculations, in order to obtain clear information about catalytic mechanisms.

University of La Sapienza **Roma, Italy**
Visiting student *February 4th, 2022-March 4th, 2022*

- Supervisor: Prof. Paola D'Angelo

- Project: Acquiring expertise in using the FDMNES package for the simulation of transition metal L edge NEXAFS spectra.

University of Trieste **Trieste, Italy**
M.Sc in Chemistry - Nanostructured and supramolecular systems *October, 2016-March, 2019*

- Attended courses: Inorganic and solid-state chemistry, Physical properties of materials, Organic materials, Ceramic materials, Advanced Physical Chemistry, Quantum Chemistry, Statistical mechanics, Chemical risk assessment, Characterization techniques with Synchrotron radiation, Computational chemistry

- Thesis title: "Core-excitation spectra of 2D boroxine-containing frameworks deposited on the Au(111) surface: a computational investigation".
  The thesis is a theoretical investigation on covalent organic frameworks deposited Au surfaces. NEXAFS spectra of B K edge have been simulated using the Amsterdam Density Functional (ADF) package, in order to interpret the experimental spectra acquired at the ALOISA beamline of Elettra Synchrotron facility (Trieste).

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- Supervisor: Prof. Daniele Toffoli
- Final grade: 110/110 cum laude
- Level 7 QEQ

University of Trieste — **Trieste, Italy**
B.Sc in Chemistry — *October, 2013-September, 2016*

- Attended courses: General chemistry, Organic chemistry, Analytical chemistry, Mathematics, Physics, Macromolecules, Biochemistry, Inorganic chemistry, Physical chemistry.
- Thesis title: "Application of DFT method to the calculation of the NEXAFS spectra of tetrazole derivatives in gas phase".
  The thesis is a theoretical investigation on tetrazole derivatives in gas phase, whose N and C K edge experimental NEXAFS spectra have been acquired on the GAS PHASE beamline of Elettra Synchrotron (Trieste). Amsterdam Density Functional (ADF) package has been used in order to simulate the spectra and interpret the experimental data.
- Supervisor: Prof. Giovanna Fronzoni
- Final grade: 109/110
- Level 6 QEQ

Liceo Scientifico Galileo Galilei — **Trieste, Italy**
High School Diploma — *September, 2007-June, 2012*

- Final grade: 91/100

WORKING EXPERIENCE

CNR IOM — **Trieste, Italy**
Research grant (assegno professionalizzante) at APE-HE beamline (Elettra Synchrotron) — *December,2022-Preser*

Main activities:

- Experimental activity mainly devoted to perform operando/in situ NEXAFS/XPS experiments on solid heterogeneous catalysts exploiting the Synchrotron radiation;
- Writing of proposals to perform experiments at other beamlines, in order to implement the results obtained at APE-HE;
- Scientific dissemination of the obtained results partecipating to workshops and conferences, writing of scientific articles;
- Experimental support as a local contact for users coming to APE-HE beamline to perform operando NEXAFS/in situ XPS experiments, for Elettra and NFFA Trieste project (`https://www.trieste.nffa.eu/people/nffa-people/silvia-mauri/`) users;
- Installation of new instrumentations and maintainance of the beamline.
- Computational simulation of NEXAFS spectra to interpret the experimental results;

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University of Trieste — **Trieste, Italy**
Tutor, Department of Life Sciences, Biochemistry I Laboratory — *October 2017 - December 2021*

- Assistence to new students;
- Tutor in biochemistry laboratories;
- Preparation of laboratory equipment.

SCIENTIFIC COMPETENCES

- **Scientific interests**: My research activity is focused on the application of X-Ray spectroscopic techniques in order to investigate the electronic structure of different kind of systems. Having matured during the years a particular interest on new materials for green energy production, I combined the two fields directing the research on the application and combination of spectroscopic techniques (in particular X-Ray absorption and photoemission spectroscopies) in operando conditions with the aim to speed up the optimization of new solid heterogeneous catalysts, exploiting a molecular-oriented approach. The theoretical formation I acquired during the B.Sc. and Master thesis complete my expertise on the above-mentioned techniques, allowing to have a complete interpretation of the data.

- **Experimental Skills and characterization techniques:**
  - Expertise (I have worked for more than four years on these topics on a daily basis) in:
    - Working on a beamline using Synchrotron Radiation source;
    - NEXAFS and X-Ray photoemission spectroscopy, with particular emphasis for in situ and operando conditions;
    - use and maintainance of UHV experimental setups;
    - Manipulation of samples in Glove box;
    - Gas chromatography (I use a micro-GC for the operando NEXAFS measurements);
    - Mass spectroscopy (I installed and used a mass spectrometer for the operando NEXAFS measurements);
  - Independent in the use of:
    - DRIFTS spectroscopy;
    - FTIR spectroscopy;
    - Scanning electron microscopy and Energy-dispersive X-ray spectroscopy (I am in charge of SEM+EDX measurements for the research group where I work i.e. APE-HE beamline);

- **Computational chemistry skills:**
  - ADF package for NEXAFS spectra simulation of light elements K edges(used for B.Sc. and Master thesis);
  - FDMNES package for NEXAFS spectra simulation of transition metal L edges;
  - CTM4XAS package for NEXAFS spectra simulation of transition metal L edges.
  - Basic knowledge of Gaussian and Quantum Espresso packages.

- **Informatics skills:**
  - Office package;

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- Data analysis softwares: Origin, Casa XPS, Demeter package;
- Molecular visualization softwares: Avogadro, VESTA;
- I combine Avogadro with 3D graphics softwares (such as Maya) in order to create scientific images for the front cover of issues related to published articles (example: `https://pubs.acs.org/cms/10.1021/jpclcd.2023.14.issue-5/asset/jpclcd.2023.14.issue-5.xlargecover.jpg`)
- Ability to work in Unix/Linux environment;
- Basic knowledge of Phyton, Fortran, Latex languages.

- **Participation to beamtimes at different european Synchrotron facilities, as main proposer or local contact**:

  - Proposal n. 20200219 (Elettra Synchrotron, APE-HE beamline) – 8-13 December 2020 – Title: Selective methanol to syngas decomposition catalyzed by Ni-Sn compounds: reaction mechanism investigation by means of operando NEXAFS spectroscopy (as **main proposer**).
  - Proposal n. 20205048 (Elettra, APE-HE beamline – 18-23 May 2021 – Title: Unveiling surface properties of GaGeTe: termination, stability and chemical reactivity (as **local contact**). Main proposer: Prof. Antonio Politano (Università degli Studi dell'Aquila).
  - Proposal n. 20210080 (Elettra, APE-HE beamline) – 13-18 September 2021 – Title: Surface termination and chemical reactivity of Pt_3Te_4 (as **local contact**). Main proposer: Daniel Farias
  - Proposal n. 20215901 (Elettra, APE-HE beamline) – 8-13 March 2022 – Title: In operando NEXAFS study of the correlation between dopant oxidation state and structure in Cu- and Fe-modified CeO_2 during H_2 dissociation (as **local contact**); Main proposer: Stefania Benedetti (Università di Modena).
  - Proposal n. 20215056 (Elettra, APE-HE beamline) – 17-22 May 2022 – Title: $AuSn_4$ and PdSn4: surface termination, chemical reactivity and ambient stability (as **local contact**). Main proposer: Chia Nung Kuo (Taiwan Consortium of Emergent Crystalline Materials, Ministry of Science and Technology, Taipei 10601, Taiwan).
  - Proposal n. 20215554 (Elettra, APE-HE beamline) - 6-11 June 2022. Title: Unveiling oxygen vacancy contribution to CO_2 fixation to Dimethyl Carbonate by in situ NEXAFS (as **local contact**). Main proposer: Davide Salusso (Università di Torino).
  - Proposal n. 20220163 (Elettra, APE-HE beamline) - 21-26 July 2022. Title: $SrTiO_3$ **A-site doped perovskites: an ambient pressure NEXAFS experiment to investigate their outstanding properties as multifunctional components for SOFCs** (as **main proposer**). Main proposer: Silvia Mauri.
  - Proposal n. 20220052 (Elettra, APE-HE beamline) - 11-16 September 2022. Title: Revealing the role of surface Sn in Ni-Sn catalysts in improving the CH_3OH selectivity to H2 at low temperatures and ambient pressure: an operando NEXAFS study on CH_3OH decomposition to syngas (H_2 + CO) (as **local contact**). Main Proposer: Danil Bouvhkalov (Ural Federal University).
  - Proposal n. 2023027289 (ALBA, CIRCE beamline) - 13-15 February 2023. Title: Cerium oxidation state in methanol oxidation by NEXAFS and Resonant photoemission (as **partecipant**). Main proposer: Virginia Pérez Dieste
  - Proposal n. SI33111 (DIAMOND LIGHT SOURCE, versoX beamline - 3-9 May 2023). Title: $SrTiO_3$ A-site doped perovskites: an in situ soft X-Rays NEXAFS experiment to investigate their outstanding properties as multifunctional components for solid oxide fuel cells (as **main proposer**).

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- Proposal n. 20225277 (Elettra Synchrotron, APE-HE Beamline - 29 May-3 June 2023). Title: An operando NEXAFS experiment to investigate the role of Cu in $CuO - BaTiO_3$ system for the selective photo-conversion of CO_2 at ambient pressure (as **Local contact**).
- Proposal n. NFFA-Trieste 2023-001 (Elettra Synchrotron, APE-HE Beamline - 25 June-3 July 2023). Title: **Structural and electronic changes of highly covalent cobalt based perovskite electrocatalysts upon water exposure** (as **Local contact**).
- Proposal n. 20230550 (MAX IV Synchrotron - SPECIES beamline, 13-18 September 2023). Title: Operando combined AP-XPS/FTIR investigation on the catalytic CH_4 activation and direct partial oxidation of Cu doped CeO_2 thin films at low temperatures (as **main proposer**).
- Proposal n. 2023027413 (ALBA Synchrotron - CIRCE beamline, 13-18 October 2023). Title: Methanol decomposition to syngas catalyzed by Ni_3Sn_4/CeO_2: combined Near Ambient Pressure XPS and NEXAFS study to investigate the role of the support in the reaction mechanism (as **main proposer**).

LANGUAGES

- **Italian** - Mother Tongue;
- **English** - Understanding: B2; Speaking: B2; Writing: B2.

PUBLICATIONS

1. Mauri, S.; Calligaro, R.; Braglia, L.; Boaro, M.; Trovarelli, A.; Torelli, P. **Low temperature methane activation over mechanochemical-induced Ce(IV)/Cu(I) interface: an in-situ DRIFT / operando NEXAFS study.** *Submitted to Nature Communications*

2. Vikatakavi A., Mauri S., Rivera-Salazar M.L., Dobovičnik E., Pelatti S., D'Addato S., Torelli P., Luches P., Benedetti S. **Role of metal dopant in hydrogen dissociation on Cu:CeO2 and Fe:CeO2 surfaces studied by ambient pressure X-ray absorption spectroscopy.** *Accepted in ACS Applied Energy Materials*

3. Taranova A., Akbar K., Yusupov K., Polewczyk V., Mauri S., Rosen J., Moras P., Moretti E., Vomiero A. **Unraveling the Optoelectronic Properties of $CoSb_x$ Intrinsic Selective Solar Absorber towards High-Temperature Surfaces.** Nat. Commun. 2023, 14, 7280. `https://doi.org/10.1038/s41467-023-42839-6`

4. Tavani F.; Busato, M.; Veclani, D.; Braglia L.; Mauri, S.; Torelli, P.; D'Angelo, P. **Investigating the High-Temperature Water/$MgCl_2$ Interface through Ambient Pressure Soft X-ray Absorption Spectroscopy** ACS Appl. Mater. Interfaces 2023, May 18. `https://doi.org/10.1021/acsami.3c02985`.

5. Mauri, S.; D'Olimpio, G.; Ghica, C.; Braglia, L.; Kuo, C.N.; Istrate, M.C.; Lue, C.S.; Ottaviano, L.; Klimczuk, T.; Boukhvalov, D.W.; Politano, A.; Torelli, P. **Hydrogen Production Mechanism in Low-Temperature Methanol Decomposition Catalyzed by Ni_3Sn_4 Intermetallic Compound: A Combined Operando and Density Functional Theory Investigation.** J. Phys. Chem. Lett. 2023,14, 13341342. `https://doi.org/10.1021/acs.jpclett.2c03471`.

6. Salusso, D; Mauri, S.; Deplano, G.; Torelli, P.; Bordiga, S.; Buzo S.R. **MOF-Derived CeO_2 and**

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$CeZrO_x$ **Solid Solutions: Exploring Ce Reduction through FTIR and NEXAFS Spectroscopy.** Nanomater. 2023, 13(2), 272; https://doi.org/10.3390/nano13020272.

7. Barreau, M.; Chen, D.; Zhang, J.; Papaefthimiou, V.; Petit, C.; Salusso, D.; Borfecchia, E.; Turczyniak-Surdacka S.; Sobczak, K.; Mauri S.; Braglia, L.; Torelli, P.; Zafeiratos, S. **Synthesis of Ni-doped ceria nanoparticles and their unusual surface reduction in hydrogen.** Mater. Today Chem. 2022, 26, 101011, ISSN 2468-5194. https://doi.org/10.1016/j.mtchem.2022.101011.

8. Tavani, F.; Busato, M.; Braglia, L.; Mauri, S.; Torelli, P.; D'angelo P. **Caught while Dissolving: Revealing the Interfacial Solvation of the Mg^{2+} Ions on the MgO Surface.** ACS Appl. Energy Mater. 2022, 14, 33, 38370–38378. https://doi.org/10.1021/acsami.2c10005.

9. Felli, A.; Mauri S.; Marelli M.; Torelli P.; Trovarelli A.; Boaro M. **Insights into the Redox Behavior of $Pr_{0.5}Ba_{0.5}MnO_{3-\delta}$ Derived Perovskites for CO_2 Valorization Technologies.** ACS Appl. Energy Mater. 2022, 5, 6, 6687–6699. https://doi.org/10.1021/acsaem.2c00163.

10. Toffoli, D.; Bernes, E.; Cossaro, A.; Balducci, G.; Stener, M.; Mauri, S.; Fronzoni, G. **Computational NEXAFS Characterization of Molecular Model Systems for 2D Boroxine Frameworks.** Nanomater. 2022, 12, 1610. https://doi.org/10.3390/nano12091610.

11. Celeste, A.; Brescia, R.; Greco, G.; Torelli, P.; Mauri, S.; Silvestri L.; Pellegrini, V.; Brutti, S. **Pushing Stoichiometries of Lithium-Rich Layered Oxides Beyond Their Limits.** ACS Appl. Energy Mater. 2022, 5, 2, 1905–1913. https://doi.org/10.1021/acsaem.1c03396.

12. Braglia, L.; Tavani, F.; Mauri, S.; Edla, R.; Krizmancic, D.; Tofoni, A.; Colombo, V.; D'Angelo, P.; Torelli, P. **Catching the Reversible Formation and Reactivity of Surface Defective Sites in Metal–Organic Frameworks: An Operando Ambient Pressure-NEXAFS Investigation.** J. Phys. Chem. Lett. 2021, 12, 37, 9182–9187. https://doi.org/10.1021/acs.jpclett.1c02585.

13. Boukhvalov, D. W.; Kuo, C. N.; Nappini, S.; Marchionni, A.; D'Olimpio, G.; Filippi, J.; Mauri, S.; Torelli, P.; Shan Lue, C. S.; Vizza, F.; Politano, A. **Efficient Electrochemical Water Splitting with PdSn4 Dirac Nodal Arc Semimetal.** *ACS Catal.* 2021, 11, 12, 7311–7318. https://doi.org/10.1021/acscatal.1c01653.

PRIZES AND AWARDS

- Winner of the "SILS Best PhD Thesis Award 'Carlo Lamberti'" at the Società Italiana Luce di Sincrotrone (SILS) Conference 2023 (August 30th-September 1st 2023, University of La Sapienza, Rome, Italy)

REVIEWING ACTIVITY FOR INTERNATIONAL SCIENTIFIC JOURNALS

- Reviewing activity for ACS Catalysis

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PARTECIPATION TO CONFERENCES

1. "Hydrogen Production Mechanism in Low-Temperature Methanol Decomposition Catalyzed by Ni3Sn4 Intermetallic Compound: A Combined Operando and Density Functional Theory Investigation". S.Mauri, G. D'Olimpio, C. Ghica, L. Braglia, C.N. Kuo, M. C. Istrate, C.S. Lue, L. Ottaviano, T. Klimczuk, D.W. Boukhvalov, A. Politano, P. Torelli. Accepted presentation at the "10th Annual Ambient Pressure X-ray Photoelectron Spectroscopy Workshop (APXPS 2023)", December 4th-8th, Taipei, Taiwan. (**Oral contribution**)

2. "Inverse CeO_2/Cu_xO catalyst for partial methane oxidation: a combined in situ DRIFT and operando NEXAFS study". S. Mauri, G. D'Olimpio, C. Ghica, L.Braglia, C.N. Kuo, M.C. Istrate, C.S. Lue, L. Ottaviano, T. Klimczuk, D. W. Boukhvalov, A. Politano, P. Torelli. S. Mauri, R. calligaro, L. Braglia, M. Boaro, F. Pauletti, S. Piccinin, S. Fabris, A. Trovarelli, P. Torelli. Accepted presentation at the "SILS Conference 2023", August 30th-September 1th 2023, Rome, Italy. (**Oral contribution**).

3. "Hydrogen Production Mechanism in Low-Temperature Methanol Decomposition Catalyzed by Ni_3Sn_4 Intermetallic Compound: A Combined Operando and Density Functional Theory Investigation". S. Mauri, G. D'Olimpio, C. Ghica, L.Braglia, C.N. Kuo, M.C. Istrate, C.S. Lue, L. Ottaviano, T. Klimczuk, D. W. Boukhvalov, A. Politano, P. Torelli. Accepted oral presentation at the EUROPACAT2023 - 15th European Conference on Catalysis, August 27th, September 1st, 2023 - Prague, Czech Republic. (**Oral contribution**)

4. "Inverse CeO_2/Cu_xO catalyst for partial methane oxidation: a combined in situ DRIFT and operando NEXAFS study". S. Mauri, R. calligaro, L. Braglia, M. Boaro, F. Pauletti, S. Piccinin, S. Fabris, A. Trovarelli, P. Torelli. Invited presentation at the "Operando soft X-ray Absorption Spectroscopy: application and perspectives" conference, July 4th-5th 2022, Trieste, Italy. (**Oral contribution**).

5. "Investigation of the surface reactivity of catalysts by operando X-ray absorption spectroscopy with Synchrotron radiation"; oral presentation at Cross-Border Workshop On Nanoscience And Nanotechnology, organized by the University of Trieste and the Jožef Stefan International Postgraduate School and Jožef Stefan Institute, 22-24 February 2022. (**Oral contribution**)

6. "Towards the understanding of the direct methane to methanol reaction mechanism catalyzed by CeO_2/Cu_xO nanomaterial: an operando NEXAFS study". Oral presentation at the New Times virtual conference, 14-18 June 2021. (**Oral contribution**)

7. "Investigation of the surface reactivity of catalysts by operando X-ray absorption spectroscopy with Synchrotron radiation"; oral presentation at Cross-Border Workshop On Nanoscience And Nanotechnology, organized by the University of Trieste and the Jožef Stefan International Postgraduate School and Jožef Stefan Institute, 23-25 February 2021. (**Oral contribution**)

8. "Towards the understanding of the direct methane to methanol reaction mechanism catalyzed by CeO_2/Cu_xO nanomaterial: an operando NEXAFS study". S. Mauri, L. Braglia, A. Petrov, G. Rossi, P. Torelli, EFCATS Summer School 2020, September 15-17, 2020, Portoroz, Slovenia. (**Oral contribution**)

9. "Towards the understanding of the direct methane to methanol reaction mechanism catalyzed by

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CeO_2/Cu_xO nanomaterial: an operando NEXAFS study". S. Mauri, L. Braglia, A. Petrov, G. Rossi, P. Torelli. Oral contribution at @CatalysisTalk organized by YEuCat (`https://www.youngcatalysis.net/`), 30 Sept. 2020. (**Invited speaker**)

10. "Revealing the role of surface Sn in Ni-Sn catalysts in improving the CH_3OH selectivity to H_2 at low temperatures". S. Mauri, G.D'Olimpio, C. Ghica, L. Braglia, C. N. Kuo, M. Cosmin Istrated, C. S. Luee, L. Ottaviano, T. Klimczuk, D. W. Boukhvalov, A. Politano, P. Torelli. CATENERCHEM winter school: "A roadmap for catalysis to support a society powered by renewable energies: Scientific and Socio-Economic Aspects of the Energy-Chemistry Nexus". March 14th-18th, 2022 - Aussois, France. (**poster presentation**).

11. "Operando Soft X-Rays Magnetic Circular Dichroism at ambient pressure: a new tool to understand the role of the spin in catalysis?". S. Mauri, L. Braglia, F. Bassato, M.L. Rivera Salazar, S. Stolfi, F. Motti, G.M. Vinai, P. Torelli. Spin matters! Magnetic order and chiral molecules in electrocatalysis workshop, 27 November 27th – 1st December 2023 - Leiden, The Netherlands. (**Poster presentation**).

SEMINARS

- "Operando Soft X-Ray Absorption Spectroscopy Applications for the Investigation of Surface Reactivity of Heterogeneous Catalysts for Methanol Valorization". S. Mauri. Invited Seminar at Ca' Foscari University (Venezia, Italy), Dipartimento di Scienze Molecolari e Nanosistemi, July 18th 2023.

PARTECIPATION TO SCHOOLS

1. EFCATS Summer School 2020, September 15-17, 2020, Portoroz, Slovenia.

2. CATENERCHEM winter school: "A roadmap for catalysis to support a society powered by renewable energies: Scientific and Socio-Economic Aspects of the Energy-Chemistry Nexus". March 14-18, 2022 - Aussois, France.

3. XVI School on Synchrotron Radiation "Gilberto Vlaic": Fundamentals, Methods and Application. September 19-30, 2022 - Muggia, Italy.

CONFERENCES AND EVENTS ORGANIZATION

- "Operando soft X-ray Absorption Spectroscopy: application and perspectives" Workshop, Trieste, 4-5 July 2022. **Partecipation at local organizing committee**, creation of the logo for the event. `https://www.trieste.nffa.eu/xas-workshop`.

SCIENTIFIC DISSEMINATION

- Trieste Next (`https://www.triestenext.it/`), 2019 and 2020 editions; Scientific dissemination to general public.
- Trieste Maker Fair (`https://trieste.makerfaire.com/`), 2020 edition;Scientific dissemination to general public.

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REFERENCES

- Dr. Piero Torelli - Laboratorio TASC, CNR-IOM (Italy) e-mail: torelli@iom.cnr.it
- Prof. Gabriele Balducci - Dipartimento di Scienze Chimiche, Università degli Studi di Trieste, via L. Giorgieri 1, 34127 Trieste; e-mail: balducci@units.it.
- Prof. Daniele Toffoli - Dipartimento di Scienze Chimiche, Università degli Studi di Trieste, via L. Giorgieri 1, 34127 Trieste; email: toffoli@units.it.

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FIRMA(**) TRIESTE, 29/02/2024

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Al di fuori dei casi sopradetti, i cittadini di Stati non appartenenti all'Unione autorizzati a soggiornare nel territorio dello Stato possono utilizzare le dichiarazioni sostitutive nei casi in cui la produzione delle stesse avvenga in applicazione di convenzioni internazionali fra l'Italia e il Paese di provenienza del dichiarante.