



Serena Esposito

Associate Professor

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Academic Position and Working Experiences

- Associate Professor of “Fondamenti Chimici delle Tecnologie” at the Department of Applied Science and Technology, Politecnico di Torino (Italy) from 16/04/2021.
- Post-Doc position in the subject area “Thin films for inorganic moisture sensors by sol-gel systems” at the Department of Materials Engineering and Production of the University of Naples "Federico II" from 1/3/2000 to 31/10/2001. Co-founded by “fondo sociale europeo-FSE programma operativo multiregionale 1994-1999
- Visiting at the University of East Anglia, Norwich (UK) under the program of “Teachers and Researchers' Mobility” in 2001. The project awarded involved the use of technology “Two dimensional HETECOR” ^1H - ^{31}P for the study of the mechanism of proton conduction in sol-gel systems $\text{P}_2\text{O}_5\text{-SiO}_2$.
- Assistant professor of “Scienza e Tecnologia dei Materiali” at the Department of Civil and Mechanical Engineering-DICEM-University of Cassino and Southern Lazio, from 2/11/2001 to 31/10/2005.
- Invited to join the unit of heterogeneous catalysis of the Department of Chemistry of the University of Parma directed by Prof. P. Moggi to test in flow-microreactors the catalytic activity of Co-SiO_2 sol-gel system in the Fisher Tropsch synthesis.
- Assistant professor of “Fondamenti Chimici delle Tecnologie” (CHIM/07) at the Department of Civil and Mechanical Engineering-DICEM University of Cassino and Southern Lazio, from 1/11/2005 to 15/02/2019.
- Visiting researcher (“congedo straordinario per motivi di studio e di ricerca” ai sensi dell’art. 8 L. 349/58, richiamato dal 1° c. art. 34 D.P.R. 382/80) in the group of Prof. Garrone- Polytechnic of Turin in 2012. She was invited to join the DISAT labs, on

account of her experience on sol-gel synthesis of catalysts, to work on catalysts for the water splitting. This invitation was encompassed in the Solhydromics project. Research activity: The role of chemistry in renewable energies; design and synthesis of catalysts for the photo-oxidative reaction of water.

- Assistant professor of “Fondamenti Chimici delle Tecnologie” (CHIM/07) Department of Applied Science and Technology (DISAT) Politecnico di Torino from 16/02/2019 to 15/04/2021.

Education

- Graduated in Chemistry (110/110 cum laude), University of Naples Federico II on July 19th 1996. The thesis entitled: "Phase transitions in a glass composition Li_2SiO_3 effect of heat treatment" was carried out in collaboration with the University of East Anglia, Norwich (UK) under the Erasmus program.
- PhD degree in Materials Engineering from the University of Naples Federico II, in February 2000, with a dissertation on "Preparation of inorganic thin films for humidity sensors using sol-gel".
- PhD visiting, two months at the University of East Anglia, Norwich (UK), working with Prof. Nigel Clayden on the Magic Angle Spinning Solid State NMR (MAS NMR) technique applied to mixed oxide systems.

Research Activity

Research activity deals with the definition of (Sol-Gel) synthesis strategies to prepare new nanostructured materials with tailored physico-chemical features. These materials find different applications spanning from heterogeneous (photo)-catalysis, energy storage & production, environmental remediation and biomedical applications.

The nanomaterials are characterized by means of several techniques, including thermal analysis, room temperature and high temperature X-ray powder diffraction, SEM and TEM microscopy, UV-visible-FTIR spectroscopy, N_2 adsorption/desorption, TPR-TPO-TPD techniques.

As testified by the authorship of publications, she has many national and international collaborations

Main research topics and their brief description

<http://www.scm.polito.it/research/>

The research activity has been always focused on the preparation and characterization of materials in the framework of applied technologies.

The preparation and characterization of glasses and glass-ceramics systems was her first research subject. After that she was fascinated from the possibility of preparing mixed oxide systems from

liquid state so she moved to the sol-gel chemistry which today she consider her main field of research. During her career she has developed an high degree of competence in the sol-gel chemistry and chemical syntheses. In particular, she developed her skills in the preparation of supported metals and metal oxide materials with tailored properties and functionalities.

As assistant prof at the University of Cassino she joined the group of Prof. Pansini, expert in zeolite systems, adding to the subjects just mentioned those concerning the use of zeolites as precursors for the preparation of ceramic phases of high technological interest and magnetic metal nanocomposites. Dealing with a bottom up approach (for materials synthesis) implies the understanding and control of the process parameters to drive the assembly of molecules and clusters into an useful structure and that was the guiding principle of her research, actually to reap the benefits of sol-gel method.

The main research topics are:

1. Sol-gel syntheses of supported metal and metal oxide catalysts →M-SiO₂, M-ZrO₂, M-TiO₂ (M= Co, Ni, Cu, Ru, Mo, Mn.). The prepared nanomaterials are studied for different applications, spanning from heterogeneous (photo)-catalysis, energy storage & production, environmental remediation.

This topic can be further subdivided into 4 sections:

a) Cobalt–silicon mixed oxide nanocomposites

Cobalt that is entrapped in a tailored matrix represents one of the most fascinating materials among the transition metal-based systems in name of its activity in many catalytic processes. To reveal the versatility of the sol-gel method, while maintaining the formation of a monolithic gel, she designed a modified hydrolytic alkoxide sol-gel route and a non-ionic surfactant assisted sol-gel route. The aim was to explore to what extent the traditional sol-gel is effective in driving the formation of specific Co phase(s), finally tailoring the catalytic features. The proposed method facilitated the introduction of hydro-soluble inorganic precursors into the synthesis medium and it led to a decrease in the gelation time with respect to the conventional alcoholic sol-gel procedure. Within a collaboration with Prof. Moggi these materials were tested as catalysts for Fischer Tropsch reaction obtaining very promising results considering that the reaction was performed in mild (P 1 bar e t 220 °C) conditions.

The comparison between the two-syntheses routes and their impact on the catalytic performance in ethanol steam reforming was also carried out thanks to a fruitful and active collaboration with the university of Milano (prof. Rossetti) and Prof. G. Ramis (university of Genova).

b) Cu-ZrO₂ catalysts for H₂ production

The preparation of copper zirconia catalysts is another example of the relevance of the

synthesis route on the performance of a catalytic material. This topic was part of a much broader research field regarding the production of hydrogen for fuel cells (proton Exchange Membrane fuel cells, PEMFC) to be used for automotive power. The oxidative steam reforming of methanol was chosen as the most performing reaction for H₂ production. The preparation has addressed some important key factors: metal dispersion, overall surface area and particles size. The catalytic results were very satisfying compared with the one reported in literature considering the lower amount of copper and the considering the absence of a promoter.

On this subject, she was speaker and chairperson at VI Italian Workshop on Sol-Gel, Lecce, June 2008. In the name of her expertise in sol-gel chemistry she was invited to organize the (next)seventh Italian Sol-Gel congress held in Naples in 2008. She is also a member of the International Sol-Gel society. Recently, she has been involved in a research concerning the preparation of mixed oxides system for the glycerol steam reforming (GSR).

On account of her expertise on sol-gel synthesis of heterogeneous catalysts, she was invited to join the group of Prof. Garrone-Polytechnic of Turin to work on catalysts for the water splitting, in the framework of an European project. Therefore, she got extraordinary leave for research purposes. Research activity: The role of chemistry in renewable energies; design and synthesis of catalysts for the photo-oxidative reaction of water. In the framework of the project, she has designed a synthesis procedure based on the emulsion method for the preparation of nanosized CoAPO-5 particles for the water splitting reaction resulting in a fourfold increase in the rate of the water oxidation reaction compared with a microcrystalline sample obtained by conventional synthesis.

c) Ru-based catalysts for green conversion of biomass

Another research activity concerns the preparation of a stable catalyst for hydrogenation reactions in the context of a broad and complex topic with a strong impact not only of a scientific nature but at industrial scale, that is the valorisation of biomass. The catalysts were tested in two important processes: the transformation of glucose in sorbitol and the formation of γ -valerolactone from levulinic acid in collaboration with Prof. Martino di Serio, University of Naples "Federico II", Department of Chemical Sciences. Notwithstanding the remarkable activity, the main concern when using ruthenium catalyst is their rapid deactivation. To overcome this obstacle, she has designed in collaboration with the research group of Prof. Antonio Aronne a one pot sol-gel procedure simple and reproducible performed at room temperature. Ru nanoparticles (ca. 3.0 nm in size) were dispersed in a Nb₂O₅-SiO₂ matrix, giving an active and stable catalyst for the levulinic acid hydrogenation to γ -valerolactone. Following a similar strategy, she has also prepared a tailored silica supported Ru catalyst by acid-catalyzed sol-gel synthesis, which proved to be a self-activating catalyst for glucose hydrogenation, showing the formation of Ru (0) lamellae not present in the pre-reduced sample. This phenomenon is certainly of great interest since it opens to the possibility of a

reduction step of the catalysts at atomic level with a glucose solution in the presence of hydrogen, a more efficient way compared with the classical packed-bed reactors approach.

d) Reverse micelle approach for mesoporous titania based (photo) catalysts

Recently she moved to the supramolecular templating sol-gel technique as an alternative approach to overcome the obstacles encountered in the most traditional procedures where the high hydrolysis rate makes the handling of transition metal alkoxides not straightforward. By the reverse micelle sol-gel approach, she has prepared mesoporous titania based nanomaterials as photocatalysts for the abatement of organic (and inorganic) water pollutants and as catalysts for the reduction of NO_x with ammonia (deNO_x reactions). Both topics are developed in the framework of national and international collaborations.

While the need for clean and sustainable methodologies has been embraced in many processes of the chemical industry more than a decade ago, such development has been significantly slower in inorganic and metal-organic synthesis. In this scenario, the rational design, based on the understanding of the key synthesis parameters, dictates their further development and application for sustainable processes. First of all, for a real green process it is important to start with a green synthesis pathway and so her first objective for the future is the design of eco-friendly protocol for synthesizing materials.

The development of synthetic routes towards the formation of multilevel porous architectures is a further challenge to optimize the properties of existing catalysts. On this topic she has recently started a collaboration with research groups at National School of Chemistry in Montpellier

Another point is that solid catalysts are usually developed in the form of divided powders. However, in the perspective of an application in industrial flow processes, the catalysts have to possess a suitable shape (in the form of extrudates, granules, pellets, or monoliths), so that high flows can be accommodated without excessive pressure drop. Recently she has published a paper reporting the comparison of the catalytic performance of commercial powder and pellets catalysts that highlight the impact of the catalysts shape on the catalytic performance. For this reason, using the flexibility and versatility of the method of sol-gel strategies for the macroscopic shaping of the materials could be a further challenge.

2. Preparation by dip-coating of thin film for gas sensors (CoO_x-SiO₂; P₂O₅-SiO₂).

She approached the sol-gel chemistry during the PhD dealing with the Sol-Gel preparation of inorganic thin films for humidity sensors. This subject was further developed during a post-doc. Within this subject, she has designed a novel synthesis approach leading to homogeneous phosphosilicate gels with chemical composition in agreement with the nominal one. Crack free thin film with high sensitivity to relative humidity were prepared by dip coating.

The correlation between the basic structure and the working mechanism is a further result of this activity achieved thanks to a research project concerning the use of the MAS-NMR tools to study the proton conduction mechanism, awarded in the framework of the program of "Teachers and Researchers' Mobility". The project was developed under the coordination of Prof. N. Clayden at the University of East Anglia, Norwich (UK), where she spent several months. The intense experimental activity on this topic has given rise to numerous works concerning phosphosilicate materials and published in the high impact ISI journal. The work was supported on behalf of National Research Council of Italy (CNR), Targeted Project "Special Materials for Advanced Technologies II" (No.980014 PF34). The results were presented in National and international congresses.

As part of a project concerning the development of advanced materials and new production technologies for applications in the field of sensors, she has designed and produced a dip-coater at the labs of the University of Cassino. The research activity involved the preparation of crack free thin film by dip coating to develop optical sensors for the detection of pollution gases. The main achievements have concerned the preparation of stable sols (CoOx-SiO₂) with different cobalt loading for the deposition of thin films, tested as optical gas sensors in collaboration with prof. Maddalena of the physics department University of Naples.

3. Preparation of metal (Fe, Ni, Fe-Co) ceramic nanocomposites for DNA separation, and toxic organic/inorganic compounds removal.

As far as the current research activity is concerned, in addition to the topic just discussed, in collaboration with Prof. Pansini (University of Cassino) she is the coordinator of a research line regarding the synthesis and characterization of magnetic metal nanocomposites.

Nanocomposites, formed by metal nanoparticles (5-25 nm) dispersed in an amorphous silica-alumina matrix, are obtained by thermal treatment in reducing atmosphere of metal exchanged zeolites. The physico-chemical properties of the nanocomposites are tailored by a wise choice of the parent zeolite and by properly tuning the thermal treatment conditions, i.e. temperature and time. The synthesis approach was patented in 2015.

The materials have been successfully applied as lunar simulants and as adsorbents for the removal of water pollutants and biomolecules.

More recently these nanocomposites have been successfully applied as magnetic adsorbents in the separation of the target gene factors V and RNASE and of the Staphylococcus aureus bacteria DNA from human blood. A possible further development is the functionalization of the nanocomposites to detect the spike (S) protein of SARS-CoV-2

4. Synthesis and structural characterization of glass and glass-ceramics with high technological applications.

The preparation and characterization of glasses has been an important research subject of

the candidate at the beginning of her career. This research has started with her Master of Science thesis carried out in cooperation with the University of East Anglia, Norwich (UK), within the Erasmus program. The use of NMR for these systems was absolutely innovative and the impact on the scientific community is testified by the high number of citations. Glass-ceramic materials containing polar phases characterized by non-linear optical activity and ferroelectric behaviour were prepared and characterized. Barium metaborate $\beta\text{BaB}_2\text{O}_4$ was studied since it shows an intense second harmonic generation (SHG), a wide transparency range and a high damage threshold. The devitrification behaviour of glasses having the stoichiometric molar ratio of barium metaborate was also studied by Fourier transform infrared (FTIR) spectroscopy, differential thermal analysis (DTA), X-ray diffraction (XRD) and scanning electron microscopy (SEM).

5. Synthesis of Alumino-silicate nanotubes.

Recently, the scientific interests extended to the synthesis of chemically modified synthetic Imogolite and methylimogolite nanotubes. Imogolite, $(\text{OH})_3\text{Al}_2\text{O}_3\text{SiOH}$ (IMO), is a naturally occurring aluminosilicate with a structure consisting of single walled nanotubes some micrometers long, with an inner diameter of ca. 1 nm and an outer diameter of ca. 2 nm. Methylimogolite, $(\text{OH})_3\text{Al}_2\text{O}_3\text{SiCH}_3$, has higher surface area, higher thermal stability and more interesting physico-chemical properties than proper imogolite NTs. She has prepared Fe-doped imogolite and methylimogolite by both direct synthesis and post synthesis methods investigating the extent of the isomorphic substitution of iron for aluminum into single-walled alumino-silicate nanotubes. Fe-doped imogolite and methylimogolite NT's are semi-conductive materials with catalytic activity in water.

Overall Scientific Production Indicators

The overall scientific production by Serena Esposito accounts for more than 85 articles on international journals, 3 book chapters, 2 patents, 1 PhD Thesis and several congress participations.

The main bibliometric parameters were evaluated on 1st August (2021):

Google Scholar: h-index 24; received citations: 1917

Scopus database: h-index 22; received citations: 1558.

Coordination of research groups

Already during PhD studies, but particularly in the following years of Post-Doctoral fellowship, contributed to the development of a research group in the field of Sol-Gel chemistry at Department of Materials Engineering and Production of the University of Naples "Federico II". She personally coordinated the activities of the research area "Thin-film by sol-gel system" and has actively

participated in the implementation of the research laboratory for what concerns the preparation and characterization of thin film by dip coating technique.

Leader of the group "Applied Nano-Materials group" (<https://sites.google.com/unicas.it/applied-nano-materials/home>) up to January 2019 at the University of Cassino and Southern Lazio.

The specific mission of the group was the preparation of porous, magnetic, ceramic or metal-ceramic nanomaterials by the sol-gel technique, controlled co-precipitation and by the thermal treatment of cation exchanged zeolites under oxidizing-inert-reducing atmosphere. Finally, the prepared nanomaterials were used in catalysis, sensors, biological separations and water remediation

Currently, she is member of the group Surf-Chem (<http://www.scm.polito.it/>) at the DISAT Department of the Politecnico di Torino. The research activity of the candidate is spread on various topic in the field of materials chemistry but particularly devoted to materials synthesis of functional materials by sol-gel process.

National and international reputation and professional activity for the scientific community

- **Reviewer** MIUR (Italian Ministry of University and Research) since 2002, since 2015 transferred to the REPRISE list (Register of Expert PeerReviewers for Italian Scientific Evaluation): Prin (Miur) projects, VQR products evaluation (Cineca), SIR projects (Miur), blue sky research unipv projects (Cineca).

- **Reviewer** European Research Council

- **Member** of the PhD school board MATERIALS SCIENCE AND TECHNOLOGY

- **Member** of the AICing (Associazione Italiana Chimica per l'Ingegneria), of the Italian Chemical Society (Industrial Chemistry Division) and affiliated to the INSTM (Istituto Nazionale di Scienza e Tecnologia dei Materiali).

- **Member** of the "International Sol-Gel Society" (ISGS).

She regularly serves as reviewers for international ISI journals: ACS journals, RSC journals, Elsevier journals, Springer journals and Wiley journals.

She is member of the board of teachers of the PhD in Materials Science and Technology at Politecnico di Torino.

She is member of the boards of teachers (Collegio dei Docenti) in mathematical engineering at the Politecnico di Torino.

Editorial roles

- **Editorial Board Members** SURFACE AND INTERFACE Elsevier ISSN: 2468-0230
<https://www.journals.elsevier.com/surfaces-and-interfaces/>

- **Associate Editor** of Chemical Reaction Engineering within FRONTIERS IN CHEMICAL ENGINEERING; Frontiers Media S.A. Country of publisher: Switzerland; 2673-2718

(Online) <https://loop.frontiersin.org/people/929988/overview>.

- **Editorial Board Member** MOLECULES, Materials Chemistry Section; MDPI (Basel, Switzerland) ISSN 1420-3049, I.F. 4.411. https://www.mdpi.com/journal/molecules/sectioneditors/materials_chemistry.
- **Editorial Board Members** MATERIALS, Catalytic Materials Section MDPI (Basel, Switzerland) ISSN: 1996-1944, IF 3.623 <https://www.mdpi.com/journal/materials/sectioneditors/catalytic>
- **Guest Editor** Guest Editor Catalysts (ISSN 2073-4344) (<http://www.mdpi.com/journal/catalysts>) Special Issue "Photocatalysts for Organics Degradation"
- **Guest Editor** Materials-MDPI (ISSN 1996-1944) (<https://www.mdpi.com/journal/materials>) Special Issue "Supported Metal and Metal Oxide Catalysts by Sol-Gel Chemistry: Synthesis and Applications".

Research Projects

She was involved in the following National Research Projects

- "Development of advanced materials and new production technologies for applications in the field of sensors". Prin 2002 Project funded by MIUR (Principal Investigator Prof. BETTA Giovanni).
- "Production of nanometric yttria-stabilized zirconia powders and production of La (1-x) Sr_xMnO₃ with a low degree of agglomeration". Prin 2004 Project funded by MIUR (Principal Investigator Prof. ANTONUCCI Pier Luigi).
- "Synthesis of titanium-zirconium hydrated oxides with high micro and meso porosity and their proton conduction". Prin 2006 Project funded by MIUR (Principal Investigator Prof. TRAVERSA Enrico).
- "Development of new adsorbent materials for ANG adsorption and storage" research contract funded by ENI (contract 1117/2019. In this project, she is involved in the research activity of the WP1, concerning the production of rGO/GO reinforced MOF nanocomposites) Politecnico di Torino.
- Research agreement with the Nurex company- biotechnology and research services (Sassari Z.I. Predda Niedda Nord strada n. 3 cod. Fisc. e P. IVA n. 01689490900). Research contract: Preparation of magnetic and porous metal-ceramic nanocomposites from FeA zeolite precursor.

Patents

S. Esposito, A. Marocco, B. Bonelli, and M. Pansini, Produzione di Materiali Compositi Metallo-Ceramici Nano Strutturati da Precursori Zeolitici. Italian Patent n. MI 2014 A 000522 deposited on the 27th of March 2014.

S. Esposito, A. Marocco, B. Bonelli, and M. Pansini, PCT international application published under Number WO 2015/145230 A1 deposited on October 1st, 2015

Participation in the scientific committees of National and International Conferences

She has participated as speaker to several national and International congresses.

Member of the scientific committee to the following national and international conferences:

- Conference “Restauro e Conservazione Dei Beni Culturali: materiali e tecniche”, 3-4 October 2003 Cassino (FR) Italy.
- VII workshop italiano Sol-Gel, 17-18 June 2010 Napoli (Italy)
- 9th International Symposium on Nano & Supramolecular Chemistry, 4-7 September 2017 Napoli (Italy).
- Principal organizer VII workshop italiano Sol-Gel, 17-18 June 2010 Napoli (Italy).
- Committee member of the International Conference on Materials: Advanced and Emerging Materials, Shenzhen, Guangdong, China from 21 to 24 November 2021

Teaching activity

Oct 2001- Sep 2018 Chemistry @BSc courses in Engineering (University of Cassino)

Sep 2019- Chemistry @BSc courses in Engineering (Politecnico di Torino)

Formal responsibility of PhD courses

From 01-11-2006 al 01-11-2010 she was in charge of 3 credits teaching (Nanotechnologies applied to materials) in the PhD course in Mechanical Engineering.

Since the A.Y. 2019-2020: she is in charge of 12 h teaching for the III level PhD course “Synthesis methods to tailor the surface and the structure properties of advanced materials”.

She has been the Academic (Co)-Supervisor of the following PhD students and MSc students:

- “Traditional metal doped TiO₂ nanoparticles obtained by sol-gel templated assisted synthesis. Physico-chemical properties and catalytic applications” (32th Cycle), PhD candidate: Roberto Nasi (Politecnico di Torino).
- “Synthesis and characterization of mesoporous TiO₂” (XXXV Cycle), PhD candidate: N. Blangetti (Politecnico di Torino).

- “Development of nanocomposites with magnetic properties for nucleic acids separation from biological fluids” Master of Science in Biomedical Engineering; candidate: Marzia Radivo (Politecnico di Torino, A.Y. 2016-2017)
- “Functionalized nanomaterials for biomolecules detection” Master of Science in Materials Engineering; candidate: Giulia Di Francesco (Politecnico di Torino, A.Y. 2017-2018).
- “Synthesis and characterization of catalysts based on ceria and zirconia for energy applications” Master of Science in Mechanical Engineering; candidate: Alessandro Billè (University of Cassino and Southern Lazio, A.Y. 2016-2017).
- “Preparation by sol-gel method of micro and meso silica as adsorbent for the simazine removal from waters”; Master of Science in Civil and Environmental Engineering; candidate: Claudia Tiracorrendo (University of Cassino and Southern Lazio, A.Y. 2010-2011).
- “Design and preparation of a low-cost humidity sensor”; Master of Science in Electrical and Information Engineering; candidate: Alessio Paglia (University of Cassino and Southern Lazio, A.Y. 2006-2007).