

**UNIVERSITY OF GENOVA**

*Doctorate Course in Sciences and Technologies  
of Chemistry and Materials*

**XXXII CYCLE YEARBOOK**

The Doctoral School of Chemical and Materials Sciences and Technologies was established in 2005 to activate research doctorates in chemistry or the like. Since 2013 (XXIX Cycle) it has been transformed into one doctorate course with 5 curricula, in which 2 are run in collaboration with the Istituto Italiano di Tecnologia (IIT) (Italian Institute of Technology).

The Doctorate aims to train high quality researchers in all research fields of fundamental chemistry (analytical chemistry, physical chemistry, inorganic chemistry, organic chemistry) and applied chemistry (pharmaceutical chemistry, food and cosmetic chemistry, pharmaceutical technologies, innovative chemical processes, environmental chemistry) as well as materials science, including nanochemistry.

For this purpose, the doctorate programme is structured into five independent curricula:

- Chemical Sciences and Technologies
- Pharmaceutical, Food and Cosmetic Sciences
- Materials Science and Technology
- Nanochemistry
- Drug Discovery and Nanobiotechnologies

The research doctorates gained additional knowledge and skills to those acquired during their previous university studies. In particular, they have been trained to handle and recognize the issues related to specific research sectors, to gain and assimilate the necessary knowledge autonomously and ultimately use it productively to solve them. Furthermore, they have developed their ability to work in groups, to exchange their interdisciplinary skills and give a clear presentation of their research results in both written and verbal form. The research doctorate will therefore be an extremely flexible and versatile figure who will be able to adapt to the new scientific and technological challenges. The balance between gaining and managing skills will enable research doctorates to conduct their important research autonomously with national and multinational companies, research bodies or universities. The doctorate provides an ideal follow-up to university studies, especially for MSc graduates in the following classes LM-13 (Pharmacy and Industrial Pharmacy), LM-17 (Physics), LM-22 (Chemical Engineering), LM-53 (Materials Science and Engineering), LM-54 (Chemical Sciences), LM-71 (Sciences and Technologies of Industrial Chemistry).

### **Research structure and teaching staff**

The Doctoral Course have relied on the collaboration of 4 Departments within the University of Genoa: the Department of Chemistry and Industrial Chemistry, the Pharmacy Department, the Physics Department, the Department of Civil, Environmental and Chemical Engineering, as well as several research units of the Italian Institute of Technology. All these departments are characterized by excellent research standards and numerous collaborations with Italian and foreign industries, universities and research bodies. Besides the structures (laboratories, instrumentation, seminar rooms) provided by these departments, the Doctoral School can rely upon a large number of teaching staff who supervise the PhD students and programme lessons or seminars. All the advisors assigned have counted on substantial research funding and therefore have assured to the Ph. D. students a sufficient budget to carry out the research.

## **Internationalization**

The doctorate course is strongly committed to internationalization and favours the attendance by foreign students. Thus, for the XXXI cycle, 6 out of 18 students were foreigner (33%).

Moreover, all italian students have been strongly encouraged to spend a secondment period abroad, as stated in the following activity reports.

I hope that this "yearbook" could remain for the new Doctors as a memory of these three years dedicated to the advancement of science, and, we are sure of that, also to the improvement of their own scientific skills and human merits.

To all of them I would like to present my best wishes for a successful and gratifying career!

Adriana Saccone  
Director of the Course

## MANAGEMENT COUNCILS OF THE COURSE

The course was governed by a Board of Professors, formed by 31 members and the Director. For the XXXII cycle the board of professors was formed by:

- Tiziano Bandiera IIT
- Luca Banfi DCCI
- Antonio Barbucci DICCA
- Andrea Basso DICCI
- Angela Bisio DIFAR
- Francesco Bonaccorso IIT
- Olga Bruno DIFAR
- Maurizio Canepa DIFI
- Dario Cavallo DCCI
- Davide Comoretto DCCI
- Simona Delsante DCCI
- Maurizio Ferretti DCCI
- Paola Fossa DIFAR
- Marco Grotti DCCI
- Roman Krahne IIT
- Riccardo Leardi DIFAR
- Emanuele Magi DCCI
- Pietro Manfrinetti DCCI
- Liberato Manna IIT
- Alberto Martinelli CNR
- Orietta Monticelli DCCI
- Paolo Olivieri DIFAR
- Teresa Pellegrino IIT
- Pierpaolo Pompa IIT
- Marina Putti DIFI
- Mirko Prato IIT
- Gianguido Ramis DICCA
- Annalisa Relini DIFI
- Paola Riani DIFAR
- Renata Riva DIFAR
- Adriana Saccone DCCI
- Silvia Schenone DIFAR

## **RESEARCH ACTIVITY**

The total number of credits achieved in 3 years is 180. The research activity is the most important part of the doctorate course. Therefore, the School has decided that this activity must correspond to a minimum of 150 credits and a maximum of 160 credits.

The research and course activities of the School are held in the followings Departments: Dep. of Chemistry and Industrial Chemistry (DCCI), Dep. of Pharmacy (DIFAR), Department of Civil, Chemical and Environmental Engineering (DICCA), Department of Physics (DIFI), Italian Institute of Technology (IIT)

At the end of each year, the students presented a written report and an oral presentation on their activity, which were evaluated by the Board of Professor of the doctorate.

## **COURSEWARE**

The remaining 20 to 30 credits are divided into these categories:

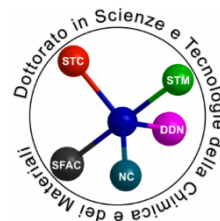
- Type A credits: short courses (4-6 hours) given by experts external to the university of Genova. Each course will have a value of 1 credit.
- Type B credits: courses given by the faculty of the School. 1 credit will correspond to 7 hours of lessons. The courses will be either of 2 or 3 credits.
- Type C credits: attendance to seminars held at the Departments involved (or in special cases also elsewhere). 1 credit corresponds to 8 seminars.
- Type D credits: participation to national or international schools for Ph.D. students. Typically, a week school will count as 2 credits.
- Type E credits: the student will prepare (also through a bibliographic search) and present a seminar on a particular subject (different from its own research work). A seminar of this kind will correspond to 2 credits.
- Type F credits: only in particular cases, when the student must fill an important gap in disciplines necessary for his/her research work, the student can be invited by the Board of Professors to attend courses activated inside one of the "master" laureas related to the subjects of the school.

Each student has chosen the distribution of these credits according the specific rules independently established by each doctorate course.



# Università degli Studi di Genova

## Doctorate in Sciences and Technologies of Chemistry and Materials



### Curriculum: Chemical Sciences and Technologies

## STEFANO ALBERTI

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*  
**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*  
**Advisor:** Prof. Maurizio Ferretti

**Thesis Title:** Sintesi, caratterizzazione, ottimizzazione e applicazione di *device* fotocatalitici a base  $\text{TiO}_2$  per applicazioni ambientali correlate all'inquinamento emergente

#### Thesis abstract

La tesi di Dottorato tratta dell'utilizzo della fotocatalisi eterogenea, in quanto Processo di Ossidazione Avanzata, per affrontare problematiche ambientali correlate all'inquinamento emergente, ossia per il trattamento di acque reflue e la decontaminazione di superfici da batteri multi-resistenti. I device fotocatalitici che verranno sintetizzati per questo progetto sono tutti a base biossido di titanio e prevedono l'accoppiamento di nanoparticelle del semiconduttore, sia tal quali che drogate, con materiali diversi, come materiali polimerici (membrane di PDMS), materiali porosi (sepioliti e zeoliti), materiali vetrosi (sferette di vetro), materiali magnetici (nanoparticelle di  $\text{Fe}_3\text{O}_4$ , zeoliti magnetiche da recupero di rifiuti industriali) e materiali a luminescenza persistente ( $3\text{ZnO}:\text{Ga}_2\text{O}_3:2\text{GeO}_2:\text{Cr}^{3+}$ ,  $\text{SrAl}_2\text{O}_4:\text{Mn}^+$  (M= Dy, Eu)). Il  $\text{TiO}_2$ , tal quale e drogato con ioni metallici e non metallici, quali ad esempio Fe, Cu, Ag o N, viene sintetizzato tramite sintesi sol-gel, mentre i materiali di supporto vengono sintetizzati tramite diverse tecniche: sintesi sol-gel, sintesi allo stato solido, sintesi idrotermale ed elettrofilatura. La sintesi di alcuni di questi campioni è stata effettuata secondo un approccio chemiometrico, ovvero utilizzando un disegno sperimentale come modello matematico per poter estrapolare le condizioni sperimentali ottimali volte ad ottenere la maggior efficienza fotocatalitica (all'interno del dominio sperimentale indagato).

I campioni sintetizzati, in base alla composizione, vengono caratterizzati dal punto di vista chimico-fisico, tramite misure di: XRD, SEM, BET, DLS, DSC, riflettanza diffusa, suscettività magnetica, prove reologiche, prove meccaniche, misure di luminescenza ed efficienza fotocatalitica. In particolare, per quest'ultima viene utilizzata la spettrofotometria UV-Vis per valutare l'abbattimento di soluzioni di blu di metilene a concentrazioni diverse (come previsto dalla norma ISO 10678:2010) e ricavarne le cinetiche dei processi. È inoltre disponibile un prototipo di impianto di trattamento dal volume processabile di 1L per effettuare valutazioni preliminari sui processi fotocatalitici nell'ottica di uno scale-up industriale. Tutti i test fotocatalitici

vengono adattati sulla base delle caratteristiche dei materiali di supporto: ad esempio, con materiali di supporto a luminescenza persistente, vengono indagate anche condizioni di buio (assenza di irraggiamento).

Infine, sono state impiegate anche tecniche cromatografiche (LC-DAD-MS, GC-FID, GC-MS) per l'identificazione e la quantificazione dei sottoprodotti di trasformazione coinvolti nei processi di abbattimento studiati.

Si può contare su collaborazioni nazionali ed internazionali, che danno credito scientifico al lavoro svolto durante il progetto: il Dipartimento di Chimica dell'Università di Pavia, che ha contribuito allo studio e allo sviluppo dei modelli chemiometrici e ai test fotocatalitici su inquinanti modello (Ofloxacin, inquinante foto-attivo modello appartenente alla famiglia degli antibiotici fluorochinolonici); il Dipartimento di Chimica dell'Università del Kuwait, nella figura del Dott. M.O. Amin, che ha contribuito allo studio sui test di recupero del fotocatalizzatore in sospensione e sulle proprietà di carica superficiale; il Dipartimento di Microbiologia dell'Università di Genova, che contribuirà allo studio delle colonie batteriche per valutazioni sull'attività antimicrobica; gli istituti CNR-IMAA e CNR-ISM, che hanno contribuito alla produzione e caratterizzazione dei materiali magnetici (zeoliti magnetiche da recupero di rifiuti) e infine il Dipartimento di Ingegneria Ambientale dell'Università Politecnica di Creta, sotto la supervisione della Professoressa E. Psillakis. In particolare, nel Water Lab della Professoressa Psillakis ho svolto parte del lavoro di dottorato: durante questo periodo, sono stati indagati gli effetti dei trattamenti di ossidazione avanzata sulla degradazione di inquinanti emergenti (parabeni, nicotina) in termini di studio sulla dipendenza del processo di ossidazione dagli effetti matrice in campioni reali e di studio dei sottoprodotti di trasformazione.

## ACTIVITY REPORT

### *Research Activity*

#### ***Research Period Abroad***

Università Politecnica di Creta, Water Lab sotto la supervisione della Professoressa E. Psillakis.

#### ***Scientific Publications***

1. Synthesis and characterization of a new photocatalyst based on TiO<sub>2</sub> nanoparticles supported on a magnetic zeolite obtained from iron and steel industrial waste, **S. Alberti**, V. Caratto, D. Peddis, C. Belviso, M. Ferretti – Journal of Alloys and Compounds 2019, 797, 820-825, DOI 10.1016/j.jallcom.2019.05.098
2. Systematic study on TiO<sub>2</sub> crystallization via hydrothermal synthesis in the presence of different ferrite nanoparticles as nucleation seeds, **S. Alberti**, S. Villa, G. Singh, F. Seland, A. Martinelli, M. Ferretti, F. Canepa, V. Caratto, Journal of Nanoscience and Nanotechnology 2019, 9:8, 4994-4999, DOI 10.1166/jnn.2019.16787
3. Porous Polydimethylsiloxane membranes loaded with low-temperature crystallized TiO<sub>2</sub> NPs for detachable antibacterial films, **S. Alberti**, M. Ferretti, S. Vicini, M. Castellano, V. Caratto - Journal of Materials Science pubblicato il 21 settembre 2018 – DOI 10.1007/s10853-018-2881-4
4. Photocatalysis in darkness. Optimization of sol-gel synthesis of NP-TiO<sub>2</sub> supported on a persistent luminescence material and its application for the removal of Ofloxacin from water. **S. Alberti**, F. Locardi, M. Sturini, A. Speltini, F. Maraschi, G.A. Costa, M. Ferretti, V. Caratto –Journal of Nanomedicine and Nanotechnology 2018, 9:3, 501– DOI 10.4172/2157-7439.1000501
5. Structural studies on copper and nitrogen doped nanosized anatase, A. Martinelli, **S. Alberti**, V. Caratto, P. Lova, F. Locardi, G. Pampararo, S. Villa, M. Ferretti currently in press in Zeitschrift fuer Kristallographie – Crystalline Materials, 2018 DOI: <https://doi.org/10.1515/zkri-2017-2143>

6. Different sol-gel preparations of iron-doped TiO<sub>2</sub> nanoparticles: characterization, photocatalytic activity and cytotoxicity, V. Caratto, F. Locardi, **S. Alberti**, S. Villa, E. Sanguineti, A. Martinelli, T. Balbi, L. Canesi, M. Ferretti – *Journal of Sol-Gel Science and Technology* (2016) 80:152–159 - DOI:10.1007/s10971-016-4057-5
7. Enhancement of TiO<sub>2</sub> NPs Activity by Fe<sub>3</sub>O<sub>4</sub> Nano-Seeds for Removal of Organic Pollutants in Water, S. Villa, V. Caratto, F. Locardi, **S. Alberti**, M. Sturini, A. Speltini, F. Maraschi, F. Canepa, M. Ferretti - *Materials* 2016, 9, 771 - DOI:10.3390/ma9090771
8. Antibacterial activity of standard and N-doped titanium dioxide-coated endotracheal tubes: an in vitro study, V. Caratto, L. Ball, E. Sanguineti, A. Insorsi, I. Firpo, **S. Alberti**, M. Ferretti, P. Pelosi - *Revista Brasileira de Terapia Intensiva*. 2017; 29(1): 55-62 – DOI:10.5935/0103-507X.20170009

#### **Oral communications:**

1. “Synthesis of a TiO<sub>2</sub>-based photocatalyst supported on a magnetic zeolite obtained from industrial waste for environmental remediation” - **S. Alberti**, V. Caratto, D. Peddis, C. Belviso, M. Ferretti - *CDCF19* - University “Sapienza” of Roma, Roma – Italy – 1-4 luglio 2019
2. “Porous PDMS membranes loaded with bare and N-doped TiO<sub>2</sub> NPs for antibacterial coatings” – **S. Alberti**, I. Basciu, A. Saperdi, S. Vicini, M. Castellano, M. Ferretti, V. Caratto - *CABC2018* - Genova – Italy, 24-27 giugno 2018
3. “Porous PDMS membranes loaded with TiO<sub>2</sub> NPs for detachable antibacterial coatings” – **S. Alberti**, I. Basciu, S. Vicini, M. Castellano, M. Ferretti, V. Caratto – *GIFC18* – Genova – Italy, 16-18 aprile 2018
4. “PDMS membranes loaded with TiO<sub>2</sub> NPs for antibacterial activity” – **S. Alberti**, V. Caratto, I. Basciu, M. Mauri, S. Vicini, M. Castellano, M. Ferretti – *ANNIC2017* – Roma, 18-20 ottobre 2017
5. “Removal of pollutants of emerging concern and the treatment of turbid wastewaters: optimization of the synthesis of NP-TiO<sub>2</sub> supported on a persistent luminescence material” – **S. Alberti**, V. Caratto, F. Locardi, M. Ferretti, G.A. Costa, M. Sturini, A. Speltini, F. Maraschi – *ICCE2017* – Oslo, 18-22 giugno 2017

#### **Poster Communications:**

1. “Synthesis and characterization of a new photocatalyst based on TiO<sub>2</sub> nanoparticles supported on magnetic materials from iron and steel industrial waste” – M. Ferretti, V. Caratto, S. Alberti, D. Peddis, M. Sturini, A. Speltini, F. Maraschi, C. Belviso – *ISMANAM2018* – Roma – Italy, 2-6 luglio 2018
2. “NPs TiO<sub>2</sub> supported on sepiolites: a photocatalytic tool for emerging pollution” – F. Fossati, S. Alberti, M. Ricci, M. Sturini, A. Speltini, F. Maraschi, V. Caratto, M. Ferretti - *CABC2018* - Genova - Italy, 24-27 giugno 2018
3. “Synthesis and characterization of a new photocatalyst based on TiO<sub>2</sub> nanoparticles supported on magnetic materials from iron and steel industrial waste” – M. Ferretti, V. Caratto, S. Alberti, P. Rizzo, D. Sangaletti, D. Peddis, M. Sturini, C. Belviso, A. Speltini - *CABC2018* - Genova - Italy, 24-27 giugno 2018
4. “PDMS membranes loaded with TiO<sub>2</sub> NPs: antibacterial activity and self-cleaning properties” - S. Alberti, V. Caratto, I. Basciu, M. Mauri, S. Vicini, M. Castellano, M. Ferretti – *CNSCI17* – Paestum, 10-14 settembre 2017
5. “Efficiency improvement of the TiO<sub>2</sub> – ZnO NPs photocatalytic coupled system supported on a persistent luminescence material” – V. Caratto, S. Alberti, G. Pampararo, F. Locardi, P. Lova, D. Comoretto, M. Sturini, F. Maraschi, A. Speltini, A. Profumo, G.A. Costa, M. Ferretti - *CNSCI17* – Paestum, 10-14 settembre 2017
6. “TiO<sub>2</sub> NPs supported on sepiolites: a photocatalytic tool for emerging pollution” – F. Fossati, S. Alberti, M. Sturini, A. Speltini, F. Maraschi, V. Caratto, M. Ferretti - *CNSCI17* – Paestum, 10-14 settembre 2017
7. “A new method for cleaning frescoes paintings” – G. Torrielli, V. Caratto, F. Fossati, S. Alberti, M. Ferretti - *CNSCI17* – Paestum, 10-14 settembre 2017



8. "Synthesis optimization and efficiency improvement of a catalytic coupled system of NPs TiO<sub>2</sub> - NPs ZnO supported on a persistent luminescence material" – P. Lova, S. Alberti, V. Caratto, F. Locardi, M. Ferretti, D. Comoretto - European Materials Research Society Fall Meeting – Varsavia, 18-21 settembre 2017.

### ***Congresses Attended***

1. "XLVII Congresso Nazionale di Chimica Fisica" - University "Sapienza" of Roma, Roma – Italy, July 1st-4th 2019
2. "XVII Congresso Nazionale di Chimica dell'ambiente e dei Beni Culturali: la tutela dell'ambiente e dei beni culturali in un mondo che cambia" – anche membro del Comitato Organizzatore – University of Genova, Genova - Italy, 24-27 giugno 2018
3. "Microinquinanti e Contaminanti Emergenti: Testimonianze, Soluzioni e Prospettive" – Polytechnic School of Milan, Milano – Italy, 11-12 giugno 2018
4. "IX Edizione delle Giornate Italo-Francesi" – Genova – Italy, 16-18 aprile 2018
5. "Applied Nanotechnology and Nanoscience International Conference" – Roma - Italy, 18-20 ottobre 2017
6. "XXVI Congresso Nazionale della Società Chimica Italiana" – Paestum, 10-14 settembre 2017
7. "16<sup>th</sup> International Conference on Chemistry and the Environment" – Oslo, 18-22 giugno 2017

## ***Courseware***

### ***Courses attended and passed:***

1. The Rietveld method: fundamentals and applications (2 CFU).
2. Industrial Catalysts and Adsorbents (2 CFU).
3. Basic scanning and transmission electron microscopies (3 CFU).
4. Experimental Design (3 CFU).
5. Synthesis, Structure and Functional Properties of Intermetallic Compounds (2 CFU).
6. Introductory course on transmission electron microscopy

### ***Courses Given by invited experts:***

1. Ivan Infante on "*DFT on Nanocrystals: Theory and Applications*", Università degli Studi di Genova, DCCI – 26-27 giugno 2019
2. Roman Krahn on "*Course on Scientific Communication Skills*", Istituto Italiano di Tecnologia – Italy, 28 ottobre e 6 dicembre 2018
3. Tiziano Tuccinardi on "*Principles of Computer-aided Drug Design*", Università degli Studi di Genova, Dipartimento di Chirurgia – Italy, 22 ottobre 2018
4. Thomas Fassler on "*Synthesis, Characterization and Properties of Intermetallic Compounds and Intermetallic Clusters*", Università degli Studi di Genova DCCI, 11 maggio 2017

### ***National and International Schools or Workshops***

1. Scuola Estiva "3<sup>rd</sup> European Summer School on Advanced Oxidation Processes", Universitat Politècnica de Valencia, - Alcoy Campus, Spain, 3-7 giugno 2019
2. Workshop "*Prima giornata di studio: Sostenibilità e processi chimici Microonde Mediat*" – Università degli Studi di Genova, DIFAR – Italy, 19 ottobre 2018
3. Workshop "*Workshop on Microactuators*", Università degli Studi di Genova, DIFI – Italy, 8 ottobre 2018

4. Workshop *AIM2018 "Advanced Inorganic Materials. Green and Unconventional Synthesis Approaches and Functional Assessment"* – University of Padova – Italy, 5-8 settembre 2018
5. Workshop *"Green Energy Applications"* con BIOLAND HOLDINGS (Cipro) – DCCI Genova, 10 maggio 2018
6. Scuola Invernale *"V Scuola di Chimica dell'Ambiente e dei Beni Culturali"* – University of Bologna, Ravenna – Italy, 22-26 gennaio 2018
7. Workshop *"PRESENCE: Phd students as a bRidge bEtween Science aNd society"*, Prof. Davide Comoretto Università degli Studi di Genova, 27 ottobre 2017
8. Workshop *"Programma PhD – La Formazione post lauream e il mondo del lavoro nell'industria Chimica, chi fa ricerca... Fa carriera?"* – Scuola Politecnica di Genova, 24 maggio 2017

### **Seminars**

1. *"Caloric Effects in Magnetic Materials"*, Prof. Hari Srikanth, Università degli Studi di Genova, DCCI – Italy, 10 settembre 2019
2. *"Insights in platinum group metal (PGM-free) catalysts for oxygen reduction reaction"*, Prof. Carlo Santoro, Università degli Studi di Genova, DCCI – Italy, 5 settembre 2019
3. *"Materiali Organici Nanostrutturati a Base Di Carbonio, Azoto e Boro"*, Paolo Giusto, Università degli Studi di Genova, DCCI – Italy, 29 novembre 2018
4. *"Anomalous transport properties in Weyl semimetals"*, Federico Cagliaris, Università degli Studi di Genova, DIFI – Italy, 19 novembre 2018
5. *"New perspectives for low temperature refrigeration with advanced magneto-caloric materials"*, Prof. Julian G. Sereni, Università degli Studi di Genova, DCCI – Italy, 13 novembre 2018
6. *"Complex Solid-Liquid Interfaces at the Nanoscale"*, Prof. Francesco Stellacci, Università degli Studi di Genova, DIFI – Italy, 31 ottobre 2018
7. *"Ligands for Functional Targeting of G-Quadruplex Nucleic Acids"*, Prof. Freccero, Università di Pavia, 7 giugno 2018
8. *"Targeting the purinergic signaling in the heart. New perspectives for understanding the electrophysiological role of adenosine in atrial fibrillation"*, PhD Luca Soattin, Cardiac Physiology Laboratory, Kobenhavns Universitet, 4 giugno 2018
9. *"Elettroni, fotoni e altre particelle"*, Prof. Luciano Maiani, DIFI Genova, 3 maggio 2018
10. *"Bi<sub>2</sub>O<sub>3</sub> ed altri composti del bismuto nella fotocatalisi: proprietà, caratteristiche e possibili nuovi spunti di ricerca"*, Prof. A. Reverberi, Università degli Studi di Genova, 29 marzo 2018
11. *"Il contributo del DCCI al Programma Nazionale di Ricerche in Antartide"*, Prof. Paola Rivaro e Prof. Marco Grotti, Università degli Studi di Genova, 27 febbraio 2018
12. *"On research activities at Muroran Institute of Technology"*, Prof. Paolo Mele, Università degli Studi di Genova, 24 luglio 2017
13. *"Analisi termica accoppiata alla gas cromatografia e spettrometria di massa. Un potente strumento per la caratterizzazione dei materiali"* - Dott. Federico Locardi, Università degli Studi di Genova, 13 giugno 2017
14. *"Sviluppo di nuovi materiali per olografia: dalla molecola al materiale"* - Dott. Andrea Bianco, Università degli Studi di Genova, 03 febbraio 2017
15. *"Fotopolimeri in astronomia: aspetti pratici e risultati in cielo"* - Dott. Alessio Zanutta, Università degli Studi di Genova, 03 febbraio 2017
16. *"Dal problema astronomico alla strumentazione: essere a metà tra scienza e tecnologia"* - Dott. Marco Landoni, Università degli Studi di Genova, 03 febbraio 2017

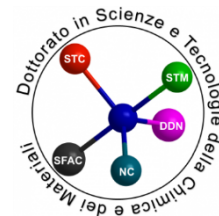
### **Other activities**

1. Referee per le riviste: Journal of Alloys and Compounds (3 lavori), Zeitschrift für Naturforschung A - A Journal of Physical Sciences (2 lavori), Journal of Materials Science (1 lavoro)

2. Incarico di collaborazione ad attività di espletamento di servizi di tutorato didattico - A\_FARM\_01 – ottobre 2019 – in corso
3. Collaborazione con l'associazione "AssoDidattica Museale" per la messa a punto di laboratori didattici presso il Museo di Chimica di Genova
4. Incarico di collaborazione con CNR-ISM sul progetto Europeo "H2020 Fetproact 2016-2017 N.731976 MAGENTA "MAGnetic nanoparticle based liquid Energy materials for Thermolectric device Application (DFM.AD003.217) – da gennaio/dicembre 2019
5. Membro della "International Advanced Oxidation Processes Ph.D School", candidato a ricevere il riconoscimento di Dottorato Internazionale sui Processi di Ossidazione Avanzata per applicazioni ambientali sull'inquinamento emergente.
6. Laboratorio didattico per studenti della scuola secondaria "Cosa mangiamo" in collaborazione con il Festival della Scienza di Cagliari, durante il Salone del Libro OFF – Torino – maggio 2018
7. Orale seminariale "Supported TiO<sub>2</sub> nanoparticles for environmental protection", S. Alberti – presentazione orale tenuta per il Workshop "Green Energy Applications" con BIOLAND HOLDINGS - 10 maggio 2018
8. Orale seminariale "Inquinamento Emergente", S. Alberti – Seminario tenuto per gli studenti del corso "Chimica Fisica Ambientale" della Laurea Magistrale in Scienze Chimiche – 20 aprile 2018
9. Membro del progetto "Porto Aperto" inteso come collaborazione tra il Dipartimento di Chimica e Chimica Industriale e l'azienda del Porto Petroli di Genova S.p.A. che offre laboratori didattici agli studenti della scuola primaria e secondaria – febbraio/maggio e ottobre/dicembre 2018
10. Incarico di collaborazione ad attività di espletamento di servizi di tutorato didattico- A\_SMFN\_04 – ottobre 2017 – febbraio 2018
11. Collaborazione nel progetto "Re-Source 4.0" per l'approvvigionamento di acqua con Unicef – novembre 2017
12. Collaborazione con il comitato organizzatore del "Mole Day" (DCCI Genova) come giornata informative per gli studenti della scuola superiore – ottobre 2017, ottobre 2018, ottobre 2019
13. Partecipazione al Workshop "Il Dottorato in Chimica. Dove siamo e dove vogliamo arrivare" – Alma Mater Studiorum, Bologna, 23 giugno 2017
14. n. 20 ore di supporto a insegnamento di "Chimica Fisica 1 con Laboratorio", cod. 65376 – Corso di Laurea in Scienza dei Materiali, Prof. M. Ferretti, 2017
15. n. 40 ore di supporto a insegnamento di "Chimica Inorganica 1 con Laboratorio", cod. 65188 – Corso di laurea in Chimica e Tecnologie Chimiche, Prof.ssa S. Delsante, 2017
16. Rappresentante degli Studenti di Dottorato nel Collegio dei Docenti, nel Consiglio e nella Giunta del Dipartimento di Chimica e Chimica Industriale (1/11/2017 – 31/10/2019)



**Università degli Studi di Genova**  
**Doctorate in**  
**Sciences and Technologies of**  
**Chemistry and Materials**



**Curriculum: Nanochemistry**

**SAHITYA KUMAR AVUGADDA**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*

**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*

**Advisors:** Dr.ssa Teresa Pellegrino (IIT), Prof.ssa Orietta Monticelli (Unige)

**Thesis Title:** Multifunctional Enzyme Responsive Nanoprobe for Theranostic applications

**Thesis abstract**

**Objective 1:** Nanoplatfrom based on iron oxide nanocubes (IONCs) coated with a bioresorbable polymer were advantageous that, upon exposure to lytic enzymes, can be disassembled increasing the heat performances in comparison with the initial clusters. As first objective, we have developed two-dimensional (2D) clusters by exploiting benchmark IONCs as heat mediators for magnetic hyperthermia and a polyhydroxyalkanoate (PHA) copolymer, a biodegradable polymer produced by bacteria that can be digested by intracellular esterase enzymes. The comparison of magnetic heat performance of the 2D assemblies with 3D centrosymmetrical assemblies or single IONCs emphasizes the benefit of the 2D assembly. Moreover, the heat losses of 2D assemblies dispersed in water are better than the 3D assemblies but worse than for single nanocubes. On the other hand, when the 2D magnetic beads (2D-MNBs) are incubated with the esterase enzyme at a physiological temperature, their magnetic heat performances began to progressively increase. After 2 h of incubation, specific absorption rate values of the 2D assembly double the ones of individually coated nanocubes. Such an increase can be mainly correlated to the splitting of the 2D-MNBs into smaller size clusters with a chain-like configuration containing few nanocubes. Moreover, 2D-MNBs exhibited nonvariable heat performances even after intentionally inducing their aggregation. Magnetophoresis measurements indicate a comparable response of 3D and 2D clusters to external magnets (0.3 T) that is by far faster than that of single nanocubes. This feature is crucial for a physical accumulation of magnetic materials in the presence of magnetic field gradients. This system is the first example of a nanoplatfrom that, upon exposure to lytic enzymes, such as those present in a tumor environment, can be disassembled from the initial 2D-MNB organization to chain-like assemblies with clear improvement of the heat magnetic losses resulting in better heat dissipation performances. The potential application of 2D nanoassemblies based on the cleavable PHAs for preserving their magnetic losses inside cells will benefit hyperthermia therapies mediated by magnetic nanoparticles under alternating magnetic fields.

**Objective 2:** - Second aim of project is to develop an assembled nanoplatfrom made of magnetic nanocubes and gadolinium-based nanoparticles (NaGdF<sub>4</sub> NPs) that makes the system responsive to tumor

microenvironment to track their tumor accumulation and enable efficient hyperthermia. For this purpose, we synthesize composite structures starting from iron oxide nanocubes (IONC) embedded in a polymeric bead with a surface negative charge (MNB) and decorated with NaGdF<sub>4</sub> NPs, placed in between enzyme-degradable polymer spacers. Our hybrid structure achieved desired heating abilities under alternative magnetic field of biological relevance. In addition to prominent T<sub>2</sub> properties, we demonstrated degradation and detaching of polymer and NaGdF<sub>4</sub> NPs from the surface of the MNBs on exposure to enzymes, that in return improved water accessibility to NaGdF<sub>4</sub> NPs with a corresponding increase in the T<sub>1</sub> signal. Indeed, we tracked the changes of the systems at different stage of the enzymatic exposure by TEM imaging. The integration of diagnostic tools to benchmark therapeutic probes could be a smart approach to enable to track the nanoparticle accumulation and improve the heat efficiency of the magnetic hyperthermia treatment at the tumor

## ACTIVITY REPORT

### *Research Activity*

#### *Research Period Abroad*

In framework of an European Compass project, I have spent **3 months** period (15/06/2018 to 15/09/2018) abroad at **Molecular foundry, Lawrence Berkley National laboratory, USA**, working on the project named. "*Automatized synthesis of magnetic mixed ferrites nanocubes and anisotropic assemblies of nanocubes for magnetic hyperthermia.*"

#### *Scientific Publications*

1. **Avugadda, S. K.** et al. Esterase-Cleavable 2D Assemblies of Magnetic Iron Oxide Nanocubes: Exploiting Enzymatic Polymer Disassembling To Improve Magnetic Hyperthermia Heat Losses. *Chem. Mater.* (2019). doi:10.1021/acs.chemmater.9b00728.
2. Dina Niculaes, Aidin Lak, George C. Anyfantis, Sergio Marras, Oliver Laslett, **Sahitya K. Avugadda**, Marco Cassani, David Serantes, Ondrej Hovorka, Roy Chantrell and Teresa Pellegrino Asymmetric Assembling of Iron Oxide Nanocubes for Improving Magnetic Hyperthermia Performance. *ACS Nano* 11, 12121–12133 (2017).
3. Materia, M. E., Leal, M. P., Scotto, M., Balakrishnan, P. B., **Avugadda, S. K.**, Garc, L., ... Pellegrino, T. (2017). Multifunctional Magnetic and Upconverting Nanobeads as Dual 2 Modal Imaging Tools 1. <https://doi.org/10.1021/acs.bioconjchem.7b00432>.

#### *Communications at Conferences*

##### *Oral communications:*

1. **Sahitya K. Avugadda**, Dina Niculaes, Maria Elena Materia, Aidin Lak , Francisco J. Teran, Ipsita Roy and Teresa Pellegrino "Assemblies of highly efficient iron oxide nanocubes for magnetic (fluid) hyperthermia to treat tumors". International Conference On Nanomedicine And Nanobiotechnology– ICONAN 2019, Munich, October 16th -18th , Germany

### **Poster Communications:**

1. **Sahitya Kumar Avugadda**, Niculaes, D., Lak, A. Controlled clustering of iron oxide nanocubes for magnetic fluid hyperthermia treatment. "Abstract Book of "16th International Conference of Nanosciences and Nanotechnologies (ICNN19) and 13th International summer school of nanoscience & Nanotechnologies 2019, Thessaloniki, Greece.
2. Barbara Salis, **Sahitya Kumar Avugadda**, Amira El Merhie, Teresa Pellegrino, Alberto Diaspro, Silvia Dante. "Interaction of nanoparticles with cellular and model membranes: influence of surface charge, size and membrane potential". International Conference On Nanomedicine And Nanobiotechnology 2018, Sept 26-28, Rome.

### **Seminars attended**

1. "Colloidal double quantum dots", Dan Oron; 14th February 2017.
2. "From cancer biology to drug treatment: Oxaliplatin in the era of personalized medicine" Paola Perego; 28th February 2017.
3. "Interplay of electronic and dynamical processes in organohalide Perovskites" Filippo De Angelis; 14th March 2017.
4. "The future of monitoring serotonin (and other neurotransmitters) in Vivo" Anne M. Andrews; 20th March 2017.
5. "Synthetic methodology for colloidal nanomaterials: limitations and opportunities", Dmitri Talapin; 26th May 2017.
6. "High-throughput design of doped colloidal nanocrystals" Speaker: Emory Chan; 1st June 2017.
7. "Perovskite nanocrystals – the new generation of defect tolerant luminescent materials", Sameer Sapra; 13th S June 2017.
8. "From Lab to the Market", Dr. Alessandro Sannino, 16th November 2017.
9. "Flat Optics Based on Metasurfaces" Prof. Federico Capasso, John A. Paulson School of Engineering and Applied Sciences, Harvard University, USA,
10. AIRC Seminar - Nanotechnology for Precision Medicine Laboratory Seminar: "Synthesis of nanostructured stimuli-responsive materials for controlled drug delivery to treat cancer". Prof. Hermis Iatrou – University of Athens
11. "Playing Lego at the nanoscale: Nanoparticles as building blocks for hierarchical structures", Pablo Guardia Department: Nanomaterials for Biomedical.
12. "Design of magnetic nano-architecture for biomedical applications", Dott. Davide Peddis, 24 gennaio 2018, Istituto di Struttura della Materia, CNR-Roma.
13. "Nanomaterials and soft polymers for implantable neural probes and artificial muscles", Christian Bergaud, PhD CNRS Researcher, LAAS - MEMS Group, Toulouse, France. Hosted by Dr. Luca Berdondini TODAY February 21<sup>st</sup> 2018.
14. "Nanoprobes for functional MRI – Towards Direct, Brain wide Recording of Neural Activity". Dr. Aviad Hai, PhD, Department of Biological Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA
15. "Engineering of iron oxide nanoparticles for magnetic particles imaging guided-hyperthermia (hMPI)", Anna C. Samia; 06th June 2018.
16. "Nanobiosensors for diagnostic applications", Arben Merkoci; 31th may 2018.

17. "Caloric Effects in Magnetic Materials", Prof. Hari Srikanth (2019 IEEE Magnetics Distinguished Lecturer University of South Florida - USA), 10 settembre 2019

## **Courseware**

### ***Courses attended and passed***

### ***Courses Given by Teachers of the Unige and IIT:***

1. Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations (1 CFU)
2. Basics of Crystallography and Diffraction by crystals (1 CFU)
3. Introductory course on transmission electron microscopy (1CFU)
4. Opto-Electronic Properties of Semiconductor Quantum Dots (1 CFU).
5. Water soluble nanoparticles (1 CFU).
6. Magnetism at the nanoscale (1 CFU).
7. Magnetic nanoparticles in nanomedicine (1 CFU).
8. Optical Spectroscopy of Colloidal Nanocrystals (1 CFU).
9. Fluorescence Super-Resolution Microscopy: Basis, Applications and Perspectives (3 CFU).

### ***Courses Given by invited experts:***

1. "An introduction to nanoscale magnetism for biomedical applications", Neil Telling, May 23rd – 24th 2017
2. "Approaches to synthesis and characterization of magnetic nanomaterials for biomedical applications", Davide Peddis
3. "From Crystallography to Imaging", Cinzia Giannini

### ***National and International Schools or Workshops***

1. 13th International Summer School on Nanosciences & Nanotechnologies Organic Electronics & Nanomedicine, Thessaloniki, Greece, 29/06/2019- 6/07/2019.
2. Workshop: "Cancer Stem Cells and Autophagy: Diagnostic and Drug Discovery" at Istituto Italiano di Tecnologia, Genova (Italy), 27 March 2017.

### ***Other Activities***

#### ***Thematic seminars***

1. NABM annual group meeting, "Assemblies of Iron oxide nanocubes for Magnetic Hyperthermia". 7th June 2017 Italian Institute of Technology.
2. NABM internal Bi-Annual meet, "Assemblies of Inorganic nanoparticles for theranostic applications" 11th December 2018 Italian Institute of Technology.
3. Sahitya kumar Avugadda, presentation for the PhD evaluation, II year, "Assembling of Inorganic nanoparticles for theranostic applications" university of Genova, October 12, 2018.
4. NABM internal meet Multifunctional magnetic gadolinium nanoprobe for theranostic application, 17th June 2019 Italian Institute of Technology.

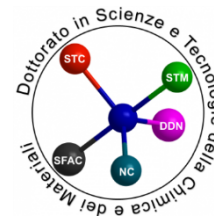
### ***Awards & Honors***

“YOUNG RESEARCHER AWARD” for best poster presentation at “13th International summer school of nanoscience & Nanotechnologies 2019”, Thessaloniki Greece.





Università degli Studi di Genova  
Doctorate in  
Sciences and Technologies of  
Chemistry and Materials



## Curriculum: Science and Technology of Materials

### MATTEO BARELLI

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*  
**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*  
**Advisor:** Prof. Francesco Buatier De Mongeot

**Thesis Title:** Plasmonics in self-organized systems

#### Thesis abstract

During my PhD program I worked on the development of self-organized bottom-up fabrication methods, aimed at the synthesis of plasmonic surfaces on large areas (square centimeter); such techniques will eventually be suitable to be adapted on the industrial scale. Plasmonic surfaces are able to increase the sensitivity of “plasmon enhanced” spectroscopies such as SERS (Surface Enhanced Raman Spectroscopy), SEIRA (Surface Enhanced InfraRed Spectroscopy) and PEF (Plasmon Enhanced Fluorescence); plasmonic surfaces are also able to amplify the photonic harvesting in new generation optoelectronic devices (thin film devices) in photovoltaics, photonics and photocatalysis.

## ACTIVITY REPORT

### *Research Activity*

The research was mainly carried out at the Department of Physics of the University of Genova

#### *Scientific Publications*

1. Maria Caterina Giordano, Stefano Longhi, **Matteo Barelli**, Francesco Buatier de Mongeot and Giuseppe Della Valle, “Plasmon hybridization engineering in self-organized anisotropic metasurfaces”, *Nano Research*, 11(7), 2018; DOI: <https://doi.org/10.1007/s12274-018-1974-3>.
2. **Matteo Barelli**, Diego Repetto and Francesco Buatier de Mongeot, “Infrared Plasmonics via Self-organized Anisotropic Wrinkling of Au/PDMS Nanoarrays” *ACS Appl. Polym. Mater.* 2019, 1, 6, 1334-1340; DOI: 10.1021/acsapm.9b00138

3. M. C. Giordano, **M. Barelli**, A. Mazzanti, G. Della Valle, F. Buatier de Mongeot, "Self-organized metasurfaces enabling plasmon hybridization", Proc. SPIE 11082, Plasmonics: Design, Materials, Fabrication, Characterization, and Applications XVII, 110821K (9 September 2019); DOI: 10.1117/12.2529154
4. **M. Barelli**, A. Mazzanti, M. C. Giordano, G. Della Valle and F. Buatier de Mongeot, "Broadband birectional color routing by self-organized plasmonic nanoantennas" under submission.
5. M.C. Giordano, **M. Barelli**, J. Vogt, M. Tzschoppe, A. Pucci and F. Buatier de Mongeot, "Self-organized nanoantennas for broadband SEIRA" under submission
6. C. Mennucci, D. Chowdhury, **M. Barelli**, G. Manzato, R. Chittofrati and F. Buatier de Mongeot, "Large area multifunctional plasmonic metasurfaces by Lloyd's Interference Lithography" under submission
7. Guided crystallization of polymer thin films over nanostructured surfaces in preparation
8. Technical report, **M. Barelli** and F. Buatier De Mongeot, "Section A - RAITH Elphy Quantum EBL module on the Hitachi SU3500 electron source: calibration and spatial resolution", in the framework of the project: Progetto Compagnia di San Paolo ID ROL 9361 "Amplificazione della raccolta fotonica in dispositivi fotovoltaici nanostrutturati".

### ***Communications at Conferences***

#### ***Oral communications***

1. "Self-organized metasurfaces for plasmon-enhanced spectroscopies and color routing", International Conference on Enhanced Spectroscopies 2019, Western University (London), Canada, 17-20 June, 2019.
2. "Plasmon hybridization engineering in self-organized anisotropic metasurfaces", Materials2018, Area della Ricerca CNR Bologna, Italy, 22-26 October, 2018.
3. Selected elevator pitch talk: "Plasmon hybridization engineering in self-organized anisotropic metasurfaces". International school of Plasmonics and Nano-optics, Cetraro (CS), Italy, 15-18 June, 2018.
4. "Plasmon hybridization engineering in self-organized anisotropic metasurfaces", Plasmonica 2018, Università di Firenze, Italy, 4-6 July, 2018.
5. "Self organized flexible plasmonic arrays", Nanopatterning 2017, Università di Helsinki, Finland, 6-30 June, 2017

#### ***Poster communications***

1. Self organized flexible plasmonic arrays" poster presentation at "IVSTA- Physics at the nanoscale" International school, held in Devet Skal, Czech Republic, 12-17 June 2017
2. "Self organized flexible plasmonic arrays" poster presentation at "Plasmonica 2017" conference in Lecce, 5-7 July 2017
3. "Plasmon hybridization engineering in self-organized anisotropic metasurfaces" poster presentation at "International school of Plasmonics and Nano-optics" held in Cetraro, 15-18 June 2018

#### ***Congresses Attended***

1. "Nanopatterning 2017" conference held in Helsinki, 26-30 June 2017
2. "Plasmonica 2017" conference held in Lecce, 5-7 July 2017

3. "Plasmonica 2018" conference held in Firenze, 4-6 July 2018
4. "Materials 2018" conference held in Bologna, 22-26 October 2018
5. "International Conference on Enhanced Spectroscopies 2019", Western University (London), Canada, 17-20 June, 2019

## ***Courseware***

### ***Courses attended and passed***

#### ***Courses Given by Teachers of the Unige and IIT:***

1. Introduzione all'applicazione della spettroscopia RAMAN ai materiali (2 credits)
2. Tecniche microscopiche e spettroscopiche per l'analisi di superfici ed interfacce (3 credits)
3. Scienza delle Superfici (3 credits)
4. Fondamenti di microscopia elettronica a scansione ed in trasmissione (3 credits)

#### ***Courses Given by invited experts:***

1. An introduction to nanoscale magnetism for biomedical applications (Lecturer: Dr. Neil Telling – A type course attended at IIT)
2. Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials / Novel Materials for energy storage and conversion (Lecturer: Dr. Thomas Fässler – A type course attended at DCCI)
3. Approaches to synthesis and characterization of magnetic nanomaterials for biomedical applications (Lecturer: Dr. Davide Peddis – A type course attended at DCCI)
4. Course on scientific communication skills (Lecturer: Roman Krahné – A type course attended at IIT Morego)

### ***National and International Schools or Workshops***

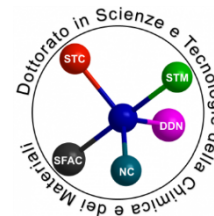
1. "IVSTA- Physics at the nanoscale" International school, held in Devet Skal, Czech Republic, 12-17 June 2017
2. "International school of Plasmonics and Nano-optics" held in Cetraro, 15-18 June 2018
3. Raith Lithography Training Course (LTC): "Electron beam lithography with Raith systems / software", held at Raith head office in Dortmund from 27/02/2018 to 01/03/2018

### ***Other Activities***

1. Attività di tutorato nell'ambito dell'attività "Formazione alla ricerca scientifica" – Stages PLS 2017, valida per orientamento all'Università e percorsi di alternanza scuola-lavoro, che si è svolta presso il Dipartimento di Fisica dell'Università degli Studi di Genova tra il 23/01/2017 e il 02/02/2017
2. Attività di tutorato nell'ambito dell'attività "Formazione alla ricerca scientifica" – Stages PLS 2018, valida per orientamento all'Università e percorsi di alternanza scuola-lavoro, che si è svolta presso il Dipartimento di Fisica dell'Università degli Studi di Genova tra il 29/01/2018 e il 08/02/2018
3. Attività di tutorato (100 ore) come tutor didattico alla pari per la Scuola di Scienze MFN da Marzo a Luglio 2019.



Università degli Studi di Genova  
Doctorate in  
Sciences and Technologies of  
Chemistry and Materials



Curriculum: Drug Discovery and Nanobiotechnologies

**ROBERTA CAGLIANI**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*  
**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*  
**Advisors:** Dr. Pier Paolo Pompa (IIT), Dr. Giuseppe Bardi (IIT), Dr. Sara Baldassari (UniGe)

**Thesis Title:** Nanobiointeractions: chemokine mediated selective targeting of nanoparticles

**ACTIVITY REPORT**

*Research Activity*

*Scientific publications*

1. **Roberta Cagliani**, Francesca Gatto, Giuseppe Bardi, Protein Adsorption: A Feasible Method for Nanoparticle Functionalization?, Materials, Published: 21 June 2019
2. Francesca Gatto, **Roberta Cagliani**, Tiziano Catelani, Daniela Guarnieri, Mauro Moglianetti, Pier Paolo Pompa, Giuseppe Bardi PMA-induced THP-1 macrophage differentiation is not impaired by citrate-coated platinum nanoparticles, Nanomaterials, Published: 17 October 2017
3. Andrea P. Falanga, Pietro Melone, **Roberta Cagliani**, Nicola Borbone, Stefano D'Errico, Gennaro Piccialli, Paolo A. Netti, and Daniela Guarnieri Design, Synthesis and Characterization of Novel Co-Polymers Decorated with Peptides for the Selective Nanoparticle Transport across the Cerebral Endothelium, Molecules, Published: 6 July 2018

*Communications at Conferences*

*Poster communications*

1. Nanobiointeractions: Nanoparticle induced modulation of immune system, World Nanotechnology Conference, Dubai 15-17 Aprile 2019

## **Courseware**

### ***Courses attended and passed (B type courses)***

1. Progettazione e sviluppo di inibitori di proteina-chinasi come nuovi agenti antitumorali- Silvia Schenone (Unige) (2 credits)
2. Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations- Luca de Trizio (IIT) (1 credit)
3. D3 PhD course: (6 credits)
4. Teresa Pellegrino: Inorganic nanoparticles for biological applications and their aqueous colloidal synthesis (1 credit)
5. Perspectives on bioinorganic chemistry-Serena de Negri (Unige)( 2 credits)

### ***Courses Given by invited experts (type B courses):***

1. "An introduction to nanoscale magnetism for biomedical applications", Neil Telling, Keele University, UK
2. "From Crystallography to Imaging", Cinzia Giannini – Institute of Crystallography – National Research Council – Bari – Italy
3. "Approaches to synthesis and characterization of magnetic nanomaterials for biomedical applications", Dott. Davide Peddis
4. "Principles of computer aided drug design", Prof Tiziano Tuccinardi

### ***National and International Schools or Workshops***

1. Cancer Stem Cells and Autophagy: Diagnostic and Drug Discovery
2. Summer School on Smart Nanomaterials for Drug Delivery 10th - 15th June 2018, Anacapri

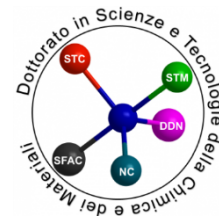
### ***Seminars***

1. NIKON@IIT Seminar: "Blood proteins and their influence on nanoparticle passage of the blood brain barrier" Dr. Silke Krol, Istituto Tumori "Giovanni Paolo II" IRCCS, Bari/Fondazione IRCCS Istituto Neurologico "Carlo Besta", Milan, Italy
2. NIKON@IIT Seminar: "AE: una nuova molecola contro il cancro? Dott.ssa Teresa Pecere, Dipartimento di Medicina Molecolare dell'Università di Padova
3. Graphene labs Van der Waals assembly of 2D materials for device application Gwan-Hyoung Lee
4. NBT seminar: Molecular pathways of neurodegeneration and treatment opportunities for amyotrophic lateral sclerosis, Davide Trotti
5. NBT seminar: Spontaneous brain activity: a key for understanding the mind and the effects of diseases on the brain, Maurizio Corbetta
6. Photoactive systems for solar energy conversion, luminescence and catalysis, Prof. Nicola Armaroli, Istituto per la Sintesi Organica e la Fotoreattività, Consiglio Nazionale delle Ricerche (CNR-ISOF)
7. NBT seminar: soft polymer based chronic neural implants, Aziz Lecomte
8. D3 seminar: Dengue and Zika virus vaccines, Oscar R. Burrone
9. Colloidal double quantum dots, Dan ORON, prof. Iwan Morel

10. D3 Seminar: "From cancer biology to drug treatment: Oxaliplatin in the era of personalized medicine, Paola Perego, Molecular Pharmacology Unit, Department of Experimental Oncology and Molecular Medicine Fondazione IRCCS Istituto Nazionale dei Tumori
11. Reconstitution of centromeric DNA structure, replication and response to stress reveals new insights into chromos, Dr. Vincenzo Costanzo - DNA Metabolism Senior Group Leader IFOM - Fondazione Istituto FIRC di Oncologia Molecolare
12. NACH Seminar: "Interplay of electronic and dynamical processes in organohalide perovskites", Filippo De Angelis, Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), CNR-ISTM, Perugia, Italy
13. D3 Seminar: "Molecular mechanisms of microtubule tip tracking and centriole formation", Michel Steinmetz, Paul Scherrer Institute, Villigen, Switzerland
14. D3 Seminar: "The Future of Monitoring Serotonin (and Other Neurotransmitters) in Vivo", Anne M. Andrews, University of California, Los Angeles
15. D3 Seminar: A cross-talk between lysosome and nucleus controls cell metabolism, Prof. Andrea Ballabio, Telethon Institute of Genetics and Medicine (TIGEM), Naples, Italy
16. Single Cell Transcriptomics to Assess Lymphocytes Identity in Health and Disease, Prof. Massimiliano Pagani, Professor, Molecular Biology Department of Medical Biotechnology and Translational Medicine Università degli Studi di Milano



**Università degli Studi di Genova**  
**Doctorate in**  
**Sciences and Technologies of**  
**Chemistry and Materials**



**Curriculum: Nanochemistry**

**LAURA CAMPAGNOLO**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*

**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*

**Advisors:** Dr. A. Athanassiou (IIT), Dr. D. Fragouli (IIT), Prof. M. Ferretti (DCCI)

**Thesis Title:** Composite porous materials for the removal of organic substances from water

**Thesis abstract**

In the last decades, agricultural activity, industrial disposal, mining effluents, and the population growth are significantly affecting the water quality, which suffers from a continuously growing number of contaminants causing adverse effects on human health and aquatic systems. Therefore, specific attention has been focused on the development of effective, robust and low-cost materials and methods for water remediation. In this thesis, it will be explored the development of new composite porous materials purposed to the detection and the removal of organic substances from water. The composite porous materials will be prepared by combining polymers, of synthetic or natural origin, with organic or inorganic fillers through several techniques of fabrication such as CO<sub>2</sub>-critical point drying, freeze-drying, electrospinning, high internal phase emulsions and phase separation process. The different techniques and material components will allow to obtain materials with desired physicochemical characteristics such as porosity, wettability, chemical affinity with desired pollutants, appropriate interactions with external sources etc. which will make them suitable for specific water remediation applications. Once the composite materials are developed, depending on their nature and on the selected pollutant, their ability to remove organic substances such as dyes, drugs or pesticides via different processes e.g. adsorption, photocatalytic degradations etc. is then evaluated.

# ACTIVITY REPORT

## *Research Activity*

### *Research Period Abroad*

University of Texas at Austin, McKetta Department of Chemical Engineering, in the group of Prof. Delia Milliron. Research related to the European project entitled "Localized Surface Plasmon Resonance in Doped Semiconductor Nanocrystals (SONAR)." (17/07/2019 to 20/10/2019)

### *Scientific Publications*

1. **Campagnolo, L.**; Lauciello, S.; Athanassiou, A.; Fragouli D. (2019) "Au/ZnO Hybrid Nanostructures on Electrospun Polymeric Mats for Improved Photocatalytic Degradation of Organic Pollutants", *Water*, 11 (9), 1787, DOI: 10.3390/w11091787
2. Vásquez, L.; **Campagnolo, L.**; Athanassiou, A.; Fragouli D. (2019) "Expanded Graphite-Polyurethane Foams for Water–Oil Filtration" *ACS Appl. Mater. Interfaces*, 11 (33) 30207-30217, DOI: 10.1021/acscami.9b07907
3. **Campagnolo, L.**; Morselli, D.; Magrì, D.; Scarpellini, A.; Demirci, C.; Colombo, M.; Athanassiou, A.; Fragouli D. (2018) "Silk Fibroin/Orange Peel Foam: an Efficient Biocomposite for Water Remediation", *Advanced Sustainable Systems*, 3 (1), DOI: 10.1002/advsu.201800097
4. Morselli, D.; **Campagnolo, L.**; Prato, M.; Papadopoulou, E. L.; Scarpellini, A.; Athanassiou, A. and Fragouli D. (2018) "Ceria/Gold Nanoparticles in Situ Synthesized on Polymeric Membranes with Enhanced Photocatalytic and Radical Scavenging Activity", *ACS Appl. Nano Mater.*, 1 (10), 5601-5611 DOI: 10.1021/acsanm.8b01227
5. **L. Campagnolo**, A. Athanassiou and D. Fragouli, *Abstract title*, in "Proceedings of the Merck Young Chemists Symposium", Ed. F. Bella, L. Botta, A. Buchicchio, R. Cucciniello, A. D'Urso, A. Erba, P. Franco, E. Lenci, G. Mazzone, A. Soldà, S. Staderini, L. Triggiani, and D. Spinelli, ISBN: 978-88-86208-89-5, 73, 2017, Rome

### *Communications at Conferences*

#### *Oral communications:*

1. "Porous biopolymers for the removal of organic pollutants from water", **Laura Campagnolo**, Athanassia Athanassiou, Despina Fragouli. Merck Young Chemists Symposium in Milano Marittima (Italy), November 13th-15th 2017
2. "Silk fibroin/orange peel composite foam: an efficient adsorbent material for water remediation", **Laura Campagnolo**, Athanassia Athanassiou, Despina Fragouli. International nanoComposites Conference (IC2), ImagineNano in Bilbao (Spain), March 14th-15th 20

## *Courseware*

### *Courses attended and passed*

### *Courses Given by Teachers of the Unige and IIT:*



1. **Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations**

*Speaker: Luca de Trizio*

- Nanomaterials: Synthesis - methods and techniques I
- Nanomaterials: Synthesis - methods and techniques II
- Post-synthesis Transformations: Cation Exchange Reactions

2. **Basics of Crystallography and Diffraction by crystals**

*Speaker: Mirko Prato*

- Symmetry, lattices, crystallographic systems and space groups
- Crystallographic computing and the reciprocal lattice
- Diffraction by crystals: theory and examples

3. **Opto-Electronic Properties of Semiconductor Quantum Dots**

*Speaker: Iwan Moreels*

- Electrons in Free Space and Bulk Crystals
- Band Structure of Bulk Metals, Insulators and Semiconductors -
- Confinement in 1, 2 and 3 Dimensions
- Optical Properties of Semiconductor Quantum Dots

4. **Super-resolution Optical Fluorescence microscopy**

*Speaker: Francesca Cella Zanacchi*

5. **Spectroscopies for chemical analysis**

*Speakers: Francisco Palazon, Roman Krahne, Iwan Moreels*

- Introduction to X-ray Photoelectron Spectroscopy
- Introduction to NMR
- Introduction to Raman

6. **Mechanical properties + atomic force microscopy**

*Speakers: Luca Ceseracciu, Marco Salerno*

- Mechanical behaviour of materials: deformation mechanisms, uni-axial testing, other mechanical properties,
- Nanoindentation: fundamentals, analysis, practical applications,
- Basic atomic force microscope working modes (contact, tapping, non- contact)
- Force sensing and advanced modes (force spectroscopy, viscoelastic imaging)

7. **Water soluble nanoparticles**

*Speaker: Teresa Pellegrino*

- Water transfer protocols of inorganic nanoparticles
- An overview of characterization techniques of water soluble nanoparticles
- Cytotoxicity of nanoparticles: methods to evaluate cytotoxicity
- Fate of nanoparticles: biological transformations of inorganic nanoparticles into living cells

8. **Introductory course on transmission electron microscopy**

*Speakers: Rosaria Brescia, Zhiya Dang, Joka Buha, Roberto Marotta*

- Introduction to transmission electron microscopy
- Analytical electron microscopy
- High-resolution TEM and in-situ TEM Introduction to electron microscopy in biology, cryo (CryoEM) electron microscopy and electron tomography

9. **Preparation and characterization of polymeric materials**

*Speakers: Dr. Alejandro Heredia Guerrero and Dr. Gianvito Caputo*

### **Courses Given by invited experts (type A courses):**

1. Approaches to synthesis and characterization of magnetic nanomaterials for biomedical applications, Prof. Clemens Burda

Topics:

- Laser Spectroscopic Studies on Perovskite Materials with the goal to unravel the electronic transport properties in these materials.
- Thermal Transport Studies with the goal to examine the temperature- dependent vibrational properties that allow dissipating absorbed thermal energy.

2. Nanoparticle Chemistry for the use of Energy Conversion and Theranostics, Prof. Clemens Burda

Topics:

- An Overview of Nanoparticle Chemistry for Photocatalysis, Plasmonics, Thermoelectrics, and use as Bio-imaging agents.
- The use of Nanoparticles for Diagnosis and Targeted Therapy of Brain Cancers.

### ***National and International Schools or Workshops***

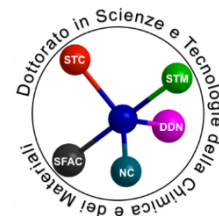
1. SINCHEM & PHOTOTRAIN Winter School, Department of Industrial Chemistry, "Toso Montanari", University of Bologna, 12th – 14th February 2018, Bologna, Italy

### ***Seminars attended***

1. Interplay of electronic and dynamical processes in organohalide perovskites, Dr. Filippo De Angelis (14/03/2017)
2. Designing and Studying Perovskite Materials for a Renewable Energy Future, Prof. Clemens Burda
3. High Throughput Electrospinning for the Design of Functional Surfaces, Nanocomposites and Barrier Structure Made of Biopolymers, Prof. Dr. Jose M. Lagaròn (31/05/2018)
4. Mapping microscale wetting variations on biological and synthetic water-repellent surfaces, Prof. Robin Ras (05/02/2018)
5. Nanoengineered surfaces and precision prototyping, Dr. Manish Kumar Tiwari (06/02/2018)
6. Nanobiosensors for diagnostics applications, Prof. Arben Merkoçi (31/05/2018)
7. Flat optics based on metasurfaces Speaker Prof. Federico Capasso (13/12/2017)
8. Precision Polymer Architectures and Conjugates to Enable Molecularly-Targeted and Cell-based Therapie, Prof. Craig Lewis Duvall (04/05/2018)
9. From Lab to the Market, Dr. Alessandro Sannino (16/11/2017)
10. Bridging the nano-gap from 1 gram to 1 tonn, Dr. Maro Bersani
11. Hollow Supramolecular Aggregates Base on Cyclic Peptides, Prof. Juan R. Granja (15/03/2019)
12. Novel plasmonic and photonic nanomaterials for optoelectronic and bio applications, Dr. Gleb Tselikov (04/03/2019)
13. Imaging in Solution: In situ liquid TEM techniques and applications, Dr. Madaline J. Dukes (22/05/2019)
14. Colloidal Copper Chalcogenide Nanocrystals: a Versatile new Class of Optoelectronic Materials, DFr. Chenghui Xia (21/11/2018)
15. Liquid crystal polymers for microrobotics and tissues engineering, Dott. Daniele Martella (24/10/2019)
16. Solid State Electrochemistry meets Power2X, Prof. Peter Holtappels (24/10/2019)



**Università degli Studi di Genova**  
**Doctorate in**  
**Sciences and Technologies of**  
**Chemistry and Materials**



**Curriculum: Drug Discovery and Nanobiotechnologies**

**FRANCESCA CARDANO**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*

**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*

**Advisors:** Prof. Silvia Giordani (IIT, Dublin City University), Prof. F. M. Raymo (University of Miami), Prof. Gabriele Caviglioli (UniGe)

**Thesis Title:** Photochromic molecular switches to assemble light-triggered drug delivery systems, sensing probes, photo-switchable polymers and to prepare photo responsive carbon-based nanomaterials

**Thesis abstract**

The thesis project is focused on the study of photochromic molecular compounds. These organic molecules show interesting chemical and physical properties that could be applied for the development of new smart applications in the nano-biotechnology field. My PhD project is focused on the study of three classes of photochromic compounds: Spiropyrans, Azobenzenes and Oxazines/Oxazolidines for several purposes. Spiropyrans are investigated for the use as light-responsive drug delivery systems due to their ability to chelate metal ions and the properties of some drugs to coordinate with cations. Azobenzenes are investigated for the design and synthesis of hybrid graphene oxide/ABs meso-structures with the prospects to obtain photo responsive materials for application in the biological realm. Oxazines and Oxazolidines photochromes are investigated in conjugation with fluorophores as coumarin and carbazole to study Temperature and pH probes and to prepare building blocks to assembly photo-switchable and modulable polymers during the research period spent as Visiting PhD student in Dr. Raymo research group.

# ACTIVITY REPORT

## *Research Activity*

### **Research Period Abroad**

- 01/10/2018-01/04/2019\_ short term scholarship at University of Miami\_ Department of Chemistry\_ Prof. Francisco Raymo Group\_Miami (USA)
- 09/10/2017-09/04/2018\_ short term scholarship at University of Miami\_ Department of Chemistry\_ Prof. Francisco Raymo Group\_Miami (USA)

### **Scientific Publications**

1. **F. Cardano**, E. Del Canto and S. Giordani. Spiropyran for light-controlled drug delivery. Dalton Trans., 2019, Advance Article DOI: 10.1039/C9DT02092F.
2. M. M.A. Mazza, **F. Cardano**, J. Cusido, J.D. Baker, S. Giordani and F. M. Raymo. Ratiometric temperature sensing with fluorescent thermochromic switches. Chem. Commun., 2019,55, 1112-1115.
3. **F. Cardano**, M. Frasconi and S. Giordani. Photo-responsive graphene and carbon nanotubes to control and tackle biological systems. Frontiers in Chemistry, 2018, 6, 102.
4. J. Sun, F. Morales-Lara, A. Klechikov, A. V. Talyzin, I. A. Baburin, G. Seifert, **F. Cardano**, M. Baldrighi, M. Frasconi and S. Giordani. Porous graphite oxide pillared with tetrapod-shaped molecules. Carbon N. Y., 2017, 120, 145-156.
5. Switchable Coumarins for Ratiometric pH Sensing\_M. M. A. Mazza, **F. Cardano**, J. D. Baker, S. Giordani and F. M. Raymo (in preparation).

## **Courseware**

### **Courses attended and passed**

#### **Courses Given by Teachers of the Unige and IIT (Type B courses):**

1. Design and synthesis of protein-kinase inhibitors as anticancer agents, Prof. Silvia Schenone\_2 CFU
2. Chimica Bio inorganica\_Prof. Serena De Negri\_2 CFU
3. Drug discovery IIT course\_6 CFU

#### **Courses Given by invited experts (Type A courses):**

1. Basics of Crystallography and Diffraction by crystals\_ IIT Nanochemistry Course (1 module in type B course)- IIT\_Dr. Mirko Prato\_1CFU
2. "Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials" and "Novel Materials for energy storage and conversion", UniGe\_Prof. Thomas Fassler\_1 CFU
3. "From Crystallography to Imaging"\_IIT\_Prof. Cinzia Giannini\_1CFU

### **Poster presentations**

1. Technological Workshop SCI\_Chemistry of graphene and applications in catalysis and polymer\_ Politecnico of Milan, Milan, 13 June 2019"Assembly of pillared graphene oxide mesostructures

2. XXXIX Convegno Nazionale della Divisione di Chimica Organica della Società Chimica Italiana, Società Chimica Italiana, University of Turin, 8-12 September 2019, "A Spiropyran Molecule for the Delivery of Aspirin".

**Schools/symposia:**

1. Mini-Symposium for PhD Students in Pharmaceutical Sciences NANOTECHNOLOGIES in PHARMACEUTICAL SCIENCES\_ University of Milan\_ 21-22-23 May 2018
2. Summer school\_COST Training School on Spectroscopy Methods for the characterization of Carbon-Related Materials\_University of Vienna\_5/8 June 2018

**Conferences attended:**

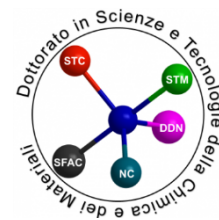
1. 27<sup>th</sup> IUPAC International Symposium in Photochemistry, University College Dublin, Dublin, 8- 13 July 2018"Photochemical and Photophysical Studies of Coumarin and Carbazole Fluorophores Conjugated with Photochromic Subunits".

**Seminars:**

1. From chemical complexity to functional complexity: tailoring multifunctional low dimensional materials and devices. P. Samorì
2. Blood proteins and their influence on nanoparticle passage of the blood brain barrier. S. Krol
3. AE: una nuova molecola contro il cancro? T. Pecere
4. Broad spectrum and subunit-specific proteasoma inhibitors and activity-based probes. H. Overkleeft
5. Van der Waals assembly of 2d materials for device applications. Gwan-Hyoung Lee
6. Molecular pathways of neurodegeneration and treatment opportunities for amyotrophic lateral sclerosis. D. Trotti
7. Photoactive systems for solar energy conversion, luminescence and catalysis. Nicola Armaroli
8. Soft polymer-based chronic neural implants. Aziliz Lecomte
9. Colloidal double quantum dots. Dan Oron
10. Dengue and Zika virus vaccines. Oscar R. Burrone
11. From cancer biology to drug treatment: Oxaliplatin in the era of personalized medicine. Paola Perego
12. Structural biopolymers – using Nature's building blocks as an inspiration for advanced manufacturing. Benedetto Marelli
13. Interplay of electronic and dynamical processes in organohalide perovskites. Filippo De Angelis
14. Molecular mechanisms of microtubule tip tracking and centriole formation. Michel Steinmetz
15. The Future of Monitoring Serotonin (and Other Neurotransmitters) in Vivo. Anne M. Andrews
16. The Roadmap to Applications of Graphene and Related Materials. Andrea Ferrari
17. Elucidation of the neurobiological and epigenetic mechanisms of disease in Kleefstra syndrome as a prelude to therapeutic intervention. Hans van Bokhoven
18. Synthesis of nanostructures and materials via self-assembly and their application to biomedical studies. Toru Maekawa



**Università degli Studi di Genova**  
**Doctorate in**  
**Sciences and Technologies of**  
**Chemistry and Materials**



**Curriculum: Nanochemistry**

**CANSUNUR DEMIRCI**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*  
**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*  
**Advisors:** Prof. Liberato Manna (IIT), Dr. Dipak Shinde (IIT),  
Prof. Simona Delsante (UniGe)

**Thesis Title:** Metallic Nanoparticles and their Application in Different Aspects of Heterogeneous Catalysis for Environmental Sciences

**Thesis abstract**

The present thesis aims the development of different catalytic materials and reaction conditions to understand the role of metallic nanoparticles in heterogeneous catalysis for environmental sciences and carbon neutrality. To do so, we will focus on three different but interdependent projects which finally result in a closed circle of emitted greenhouse gas (carbon dioxide CO<sub>2</sub> and methane CH<sub>4</sub>) regulation. In a first project we focused on the controlled selectivity of the oxidative coupling of methanol to methyl formate, in which CO<sub>2</sub> is an undesirable side product. In this project we decided to study the role of metal traces in a nanoporous gold system to study their influence in the activity but also selectivity of the reaction. In a second project, we focused on the controlled combustion of methane in vehicle exhausts to form the less harmful greenhouse gas CO<sub>2</sub>. In this project we aimed to increase the activity of a palladium catalyst (Pd-nanoparticles on an alumina support) by applying a higher total pressure to avoid methane slips during the vehicle combustion process (in case of natural gas vehicles). In the third and last project, we aimed the caption of CO<sub>2</sub>, by reducing it electrochemically on a copper catalyst to obtain products involving one to three carbon atoms. By decorating the copper catalyst with increasing amounts of gold, the selectivity but also reactivity of the catalyst was further studied. Finally, this comprehensive thesis combines work from different fields of catalysis, showing how different and varied each section is, yet also highlighting their interdependencies to obtain a holistic working method of a carbon neutral process.

# ACTIVITY REPORT

## *Research Activity*

### *Research Period Abroad*

September 2018 – February 2019: Research stay at Chalmers University of Technology, Gothenburg, Sweden, Host Professor Magnus Skoglundh (Head of Competence Centre for Catalysis at Chalmers University of Technology)

### *Scientific Publications*

1. **Demirci, C.**, Marras, S., Prato, M., Pasquale, L., Manna, L. Massimo, C., Design of catalytically active porous gold structures from a bottom-up method: The role of metal traces in CO oxidation and oxidative coupling of methanol, *J. Catal.*, 2019, 375, 279-286.  
<https://doi.org/10.1016/j.jcat.2019.06.016>.
2. Florén, C.-R., **Demirci, C.**, Carlsson, P.-A., Creaser, D., Skoglundh, M., Total oxidation of methane over Pd/Al<sub>2</sub>O<sub>3</sub> at pressures from 1 to 10 atm, (submitted to *Chemical Engineering Journal*).
3. Bellani, S., Martín-García, B., Oropesa-Nuñez, R., Romano, V., Najafi, L., **Demirci, C.**, Prato, M., Del Rio Castillo, A. E., Marasco, L., Mantero, L., D'Angelo, G., Bonaccorso, F., "Ion sliding" on graphene: a novel concept to boost supercapacitor performance, *Nanoscale Horiz.*, 2019, 4, 1077-1091. <https://doi.org/10.1039/C8NH00446C>
4. Campagnolo, L., Morselli, D., Magrì, D., Scarpellini, A., **Demirci, C.**, Colombo, M., Athanassiou, A., Fragouli, D., Silk Fibroin/Orange Peel Foam: An Efficient Biocomposite for Water Remediation, *Adv. Sustainable Syst.* 2019, 3, 1800097. <https://doi.org/10.1002/adsu.201800097>

### *Communications at Conferences*

#### *Poster Communications:*

1. Presented at Catalysis Fundamentals and Practice Summer School, Liverpool (United Kingdom) 17-21 July 2017
2. Presented at Faraday Discussion: Designing Nanoparticle Systems for Catalysis, London (United Kingdom), 16-18 May 2018
3. Presented at EuropaCat: Catalysis without Borders, Aachen (Germany), 18-23 August 2019

#### *Oral Communications:*

1. Presented at Faraday Discussion: Designing Nanoparticle Systems for Catalysis, London (United Kingdom), 16-18 May 2018

## **Courseware**

### ***Courses attended and passed***

#### ***Courses Given by Teachers of the Unige and IIT:***

1. Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations (1 CFU) – Luca De Trizio (1 credit)
2. Basics of Crystallography and Diffraction by crystals (1 CFU) – Mirko Prato (1 credit)
3. Introductory course on transmission electron microscopy– Rosaria Brescia, Roberto Marotta, Zhiya Dang, Joka Buha (1 CFU)
4. Spectroscopies for chemical analysis (1 CFU) - Francisco Palazon, Roman Krahné, Iwan Moreels
5. Mechanical properties + atomic force microscopy – Luca Ceseracciu, Marco Salerno, (1 credit)
6. Water soluble nanoparticles– Teresa Pellegrino (1 CFU)
7. Optical Spectroscopy of Colloidal Nanocrystals– Dmitry Baranov (1 credit)
8. Optical properties of low-dimensional materials, Ilka Kriegel (1 CFU)

#### ***Type A Courses Given by invited experts:***

1. “Challenges in chemical synthesis for energy storage and energy conversion materials”, and “Novel materials for energy storage and conversion” by Prof. Dr. Thomas Fässler
2. “An introduction to nanoscale magnetism for biomedical applications, Session 1: Magnetism and the nanoscale; Session 2: Biomedical applications of magnetic nanoparticles”, by Neil Telling
3. “From Crystallography to Imaging”, by Cinzia Giannini
4. “Probing Matter with Synchrotron Radiation” by Luigi Paolasini

#### ***National and International Schools or Workshops***

1. Catalysis Fundamentals and Practice Summer School, Liverpool (United Kingdom), 17-21 July 2017
2. International Spring School of Electrochemistry, Castellammare del Golfo (Italy), 19-23 May 2019

#### ***Seminars***

1. “Interplay of electronic and dynamical processes in organohalide perovskites” by Filippo de Angelis
2. “High-throughput-design of doped colloidal nanocrystals” by Emory Chan
3. “Application of nanocrystals to photo catalysis and exhaust gas purification” by Dr. Takahiro Ikeda
4. “Synthetic methodology for colloidal materials: Limitations and opportunities” by Dmitri Talapin
5. “Integrated photo electrodes for CO<sub>2</sub> reduction and water oxidation” by Francesca M. Toma
6. “Flat optics based on meta surfaces” by Prof. Federico Capasso
7. “The physics of the universe, over more than 60 orders of magnitude of length” by Antonio Ereditato
8. “Aberration-corrected STEM: sub-Å resolution imaging, atomic resolution elemental mapping, and vibrational spectroscopy” by Ondrej L. Krivanek
9. “Standardization methods for synthesis of single-core and multi-core magnetic nanoparticles for medical applications” by Helena Gavilan Rubio
10. “One-year stable perovskite solar cells by 2D/3D interface engineering” by Dr. Giulia Grancini
11. “Membrane engineering” by Dr. Enrico Drioli



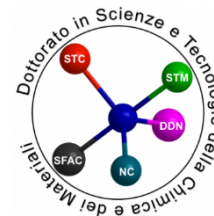
12. "Colloidal semiconductor nanocrystals" by Ivan Infante
13. "Scattering-Type Scanning Near-Field Optical microscopy for various applications" by Dr. Philip Schaefer
14. "Nonlinear nanophotonics with 2d materials and near-zero index media" by Andrea Marini
15. "Some Strategies to Integrate Graphene into Functional Materials" by Mildred Quintana
16. "We Play with Chemistry to Design Colloidal Semiconductor Nanocrystals" by Vladimir Lesnyak

### ***Other Activities***

1. Measurement at Synchrotron Facilities: Soleil Synchrotron, ROCK Beamline, Saint-Aubin, France, 21 – 25 March 2018
2. Measurement at Synchrotron Facilities: Paul Scherrer Institut, Swiss Light Source, Beamline Super-XAS, Villigen, Switzerland, 5-11 June 2018
3. YEuCat: Involved in kick-off phase (since August 2019) for a society/ group of young scientists in catalysis in Europe, Task: Organization of group members and their visualization on an online map. <https://www.youngcatalysis.net/>



**Università degli Studi di Genova**  
**Doctorate in**  
**Sciences and Technologies of**  
**Chemistry and Materials**



**Curriculum: Pharmaceutical, Food and Cosmetic Sciences**

**ROMEO ARAGO – DOUGUE KENTSOP**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*

**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*

**Advisors:** Prof.ssa Angela Bisio, Dott.ssa Barbara Ruffoni

**Thesis Title:** Biotechnology applied to aromatic plants for the controlled production of bioactive compounds

## **ACTIVITY REPORT**

### ***Research Activity***

#### ***Research Period Abroad***

- Discontinuous periods from 1<sup>st</sup> November 2016 to 31<sup>st</sup> October 2019 at CREA-OF (Consiglio per la ricerca in agricoltura e l'analisi dell'economia agraria- Orticoltura e Florovivaismo) Sanremo (IM).
- Research period from 8<sup>th</sup> April to 22<sup>nd</sup> May 2019 at the Pharmacy Department of the University of Fisciano (SA).

#### ***Communications at Conferences***

##### ***Oral communications***

1. Establishment of Hairy Root Cultures of *Salvia corrugata* Vahl. for Biomass Production. Riunione Annuale dei Gruppi di Lavoro SBI Biologia Cellulare Molecolare biotecnologie e differenziamento 13th to 15th Giugno 2018, Sanremo, Italia.
2. Production of biopharmaceutical proteins: particular case of Plant, Seminari dei dottorandi del XXXII° ciclo, 15 ottobre 2019, (DIFAR)
3. Biotechnology for the production of bioactive metabolites in *Salvia corrugata* Vahl, Seminario CREA 2019, Centro di Ricerca Orticoltura e Florovivaismo, 16 ottobre, Sanremo (IM), Italia.

### **Poster communications**

1. Angela Bisio, Francesca Pedrelli, **Roméo Arago Dougué Kentsop**, Barbara Ruffoni, Nunziatina De Tommasi, Anna Maria Schito, *Antimicrobial activity of Salvia tingitana Etl. (Lamiaceae)*, XV Congress of the Italian Society of Phytochemistry and 1<sup>st</sup> International Congress on Edible, Medicinal and Aromatic Plants (ICEMAP 2017), 28-30 June 2017, Pisa, Italy.
2. Angela Bisio, Francesca Pedrelli, **Romeo Arago Dougué Kentsop**, Daniele Fraternali, Barbara Ruffoni, Nunziatina De Tommasi, Anna Maria Schito, *Antibacterial activity of roots of Salvia corrugata Vahl*, 112° Congresso della Società Botanica Italiana, IV International Plant Science Conference (IPSC). Parma Campus Universitario 20 - 23 September 2017.
3. **Roméo Arago Dougué Kentsop**, Elena Lazarova, Francesca Pedrelli, Marco Savona, Martina Fabiano, Mauro Giacomini, Barbara Ruffoni, Anna Maria Schito, Nunziatina De Tommasi, Angela Bisio, *Establishment of hairy root cultures of Salvia corrugata Vahl*, XVI Congress of the Italian Society of Phytochemistry jointly with 2<sup>nd</sup> International Congress on Edible, Medicinal and Aromatic Plants (ICEMAP 2019), 19-21 June 2019, Alghero (ss) Italy.
4. Angela Bisio, Francesca Pedrelli, **Roméo Arago Dougué Kentsop**, Massimiliano D'Ambola, Martina Fabiano, Barbara Ruffoni, Gabriella Piatti, Gian Carlo Schito, Nunziatina De Tommasi, Anna Maria Schito, *Antibacterial activity of abietane diterpenes from the root and hairy roots of Salvia corrugata Vahl*, 67<sup>th</sup> International Congress and Annual Meeting of the Society for Medicinal Plant and Natural Product Research (GA 2019), 1st al 5th September 2019, Innsbruck, Austria.
5. Bisio Angela, Francesca Pedrelli, Martina, Fabiano, **Roméo Arago Dougué Kentsop**, Gian Carlo Schito, Anna Maria Schito, Nunziatina De Tommasi, *Abietane Diterpene constituents from the roots of Salvia tingitana Etl. (Lamiaceae)*, 114° Congresso della Società Botanica Italiana, VI International Plant Science Conference (IPSC) e 11° Congresso Annuale della Società Italiana di Biologia Vegetale, 4 - 7 September 2019, Padova, Italy.

### **Congresses Attended**

1. 65<sup>th</sup> International Congress and Annual Meeting of the Society for Medicinal Plant and Natural Product Research (GA 2017), 3rd to 7th September 2017, Basel, Switzerland.
2. Riunione Annuale dei Gruppi di Lavoro SBI Biologia Cellulare Molecolare biotecnologie e differenziamento 13th to 15th Giugno 2018, Sanremo, Italia
3. pHealth 2019 16th International Conference on Wearable, Micro & Nano technologies for Personalized Health, 10 to- 2 June 2019, Genoa, Italy.
4. XVI Congress of the Italian Society of Phytochemistry jointly with 2<sup>nd</sup> International Congress on Edible Medicinal and Aromatic Plants (ICEMAP 2019), 19 to 21 June 2019 Hotel Catalunya – Sala Convegni, Alghero (SS) Italy.
5. 67<sup>th</sup> International Congress and Annual Meeting of the Society for Medicinal Plant and Natural Product Research (GA 2019), 1st to 5th September 2019, Innsbruck, Austria.

### **Courseware**

#### **Courses passed**

1. Pharmaceutical Biotechnology given by Prof. M. Mazzei (3 credits)
2. Innovative pharmaceutical dosage forms: preparation and control methods given by Prof. S. Baldassari, G. Caviglioli, G. Zuccari and E. Russo (2 credits)
3. Experimental Design given by Prof. M. Grotti and R. Leardi (3 credits)
4. Principal plants used in Phytocosmetics and their constituents given by Prof. A. Bisio (2 credits)

5. Patent and bibliographic databases searching in medicinal chemistry given by Prof. P. Fossa and C. Brullo (2 credits)
6. Instrumental techniques for trace elements determination in pharmaceuticals, food products and environmental samples given by Prof. V. Minganti and G. Drava (2 credits)

#### ***Courses Given by invited experts:***

1. "Organic Synthesis and Catalysis in the Pharmaceutical Industry", Dott. Paolo Tosatti, Senior Scientist, Roche, Basel, Venerdì, 20 settembre 2019, DCCI
2. "New Trends in Computer-aided Drug Design", Prof. Tiziano Tuccinardi, 7 October 2019, Polo Biomedico Ex Saiwa

#### ***National and International Schools or Workshops***

1. The Nagoya Protocol: access and benefit-sharing of nature's genetic resources. Florence, 27th February 2017 –Rectorate of Florence University – Piazza San Marco
2. Scuola "Paolo Cecherelli" Filiera corta in campo erboristico e medicinale; sviluppo tecnologico e programmazione comunitaria, Albenga 7-9 giugno 2018
3. African Research Workshop: 67th international congress and annual meeting of the society for medicinal plant and natural product research (GA 2019), 1st - 5th September 2019, Innsbruck, Austria.

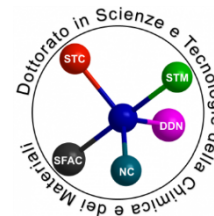
#### ***Seminars***

1. "Technical seminar on innovation of products made of aromatic plants". Sanremo (Italy), 13th April 2017
2. "Il fascino dell'impollinazione forme, colori e odori, che utilizzano i fiori per attrarre gli impollinatori". 18 Maggio 2017 presso CREA, Sanremo (Imperia)
3. "33mo Incontro fitoiatrici – Nuovo problemi e prospettive di soluzione nel settore delle colture ornamentali". 27 Settembre 2017, Floriseum – Villa Ormond – Sanremo (IM)
4. "Novel Small Molecules, Targets, and Strategies in Anti-infective Development", Prof. Jason K. Sello, Ph.D., Department of Chemistry Brown University 3 Luglio 2017, Genova, DCCI
5. "Dalle origini ai giorni nostri (the vaccines: from the origins to the present day)", Sanna Monica. 2017, DIFAR, Seminari dei dottorandi del XXX° ciclo.
6. "Chronic Obstructive pulmonary Disease (COPD)", Brignole Daniele, 2017. DIFAR, Seminari dei dottorandi del XXX° ciclo.
7. "Imagining in Oncology" Pastorino Sara. 2017, (DIFAR- viale BenedettoXV). Seminari dei dottorandi del XXX° ciclo.
8. "Depression: new therapeutic strategies" Sadeghi Mohamed, 2017, DIFAR- Seminari dei dottorandi del XXX° ciclo
9. "Probiotics: properties, use and interaction with human microbiome" Turrini Federica. 2017, (DIFAR), Seminari dei dottorandi del XXX° ciclo
10. "Il Rosmarino i segreti di una pianta comune", 24 Marzo 2018 Floriseum – Villa Ormond – Sanremo (IM)
11. "Hippeastrum stella dei cavalieri", 07 Aprile 2018 Floriseum – Villa Ormond – Sanremo (IM)
12. "La cooperazione al cuore del Mediterraneo", Seminario sull'ulivo svoltosi. Centro di Ricerca Orticoltura e Florovivaismo (CREA-OF) Sanremo, 23 ottobre 2018

13. "Il comparto floricolo e vivastico della Campania: il punto di vista dei produttori", presentato da Luigi D'Amora, Domenico Sabatino e Marco Scognamiglio – Cooperativa Campana la Nuova Floricoltura Meridionale, in collegamento web dal Centro di Ricerca Orticoltura e Florovivaismo (CREA-OF), sede di Pontecagnano Faiano, 2 ottobre 2019
14. "Biocatalysis in medicinal chemistry". Dott.ssa Erika Tassano (Novartis Pharma AG, Basilea, Svizzera), 4 ottobre - Dipartimento di Chimica e Chimica Industriale.
15. "Astrochemistry: The chemistry of stars", Valeria Francesconi, Seminari dei dottorandi del XXXII° ciclo (DIFAR)
16. "Preliminary in vitro essays to evaluate anticancer drugs", Chiara Greco, Seminari dei dottorandi del XXXII° ciclo (DIFAR)
17. "Design of Experimental: Full Factorial Design and Case Study", Maryam Hooshyari, Seminari dei dottorandi del XXXII° ciclo (DIFAR)
18. "Combination of conventional antibiotics with natural products: a promising strategy in overcoming antibiotic resistance" Francesca Pedrelli, Seminari dei dottorandi del XXXII° ciclo, 15 ottobre 2019 (DIFAR)



**Università degli Studi di Genova**  
**Doctorate in**  
**Sciences and Technologies of**  
**Chemistry and Materials**



**Curriculum: Nanochemistry**

**SERGIO FIORITO**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*  
**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*  
**Advisors:** Dr. Teresa Pellegrino (IIT), Prof. Fabio Canepa (UniGe)

**Thesis Title:** Iron oxide-gold-copper sulfide nano-heterostructures: a novel multidomain platform for theragnostic applications

**Thesis abstract**

The goal of the Ph.D. research activity was to develop inorganic heterostructures able to be used in different theragnostic applications. In particular, the research activity has been focused to the development of structures able to be used both in magnetic hyperthermia and as radioisotope carriers for radiotherapy or positron emission tomography (PET).

The research group where the activity was carried on, has a strong know-how on the synthesis and functionalization of magnetic nanoparticles<sup>1-3</sup> or magnetic heterostructures<sup>4</sup> with excellent efficiency when used as heating probes in magnetic hyperthermia. Likewise, recently, the possibility to use semiconductor nanocrystals (such as CuS) as radioisotope carrier (<sup>64</sup>Cu) was demonstrated. During these three years of research activity, new materials for these purposes were developed.

First, ZnS nanoparticles were synthesized and phase transferred to water using an appropriate water-transfer procedure. These nanoparticles have been proven to be successfully radiolabeled with <sup>64</sup>Cu up to a maximum of 13% of Zn (II) ions replaced with <sup>64</sup>Cu (I) obtaining a quantitative radiolabeling (yield of ≈93%).

Different trials were performed in order to merge a semiconductor domain able to be used in radiolabeling experiments with a magnetic domain that could be used in magnetic hyperthermia. While trials to grow FexOy@ZnS or FexOy@Au@ZnS nano-heterostructures were not successful, FexOy@Au@Cu<sub>2-x</sub>S heterostructures were successfully obtained.

These FexOy@Au@Cu<sub>2-x</sub>S trimers were water transferred by developing different phase-transfer procedures and their hyperthermia and radiolabeling properties tested. Hyperthermia efficiency of the trimers in biologically safe conditions (below the H\*f limit value of 5 × 10<sup>9</sup> A/(m\*s)) is excellent and comparable with the ones obtained for iron oxide nanocubes produced by Guardia et al. FexOy@Au@Cu<sub>2-x</sub>S: S. Trimers were also quantitatively radiolabeled (radiolabeling yield >90%) with <sup>64</sup>Cu (I). Excellent efficiency both when used in magnetic hyperthermia and as material suitable to incorporate radioisotopes (<sup>64</sup>Cu), clearly identify FexOy@Au@Cu<sub>2-x</sub>S trimers as the first reported candidate material

able to merge cancer therapy with magnetic hyperthermia and radiotherapy or diagnosis through positron emission tomography.

#### REFERENCES:

1. Guardia, P. et al. Water-Soluble Iron Oxide Nanocubes with High Values of Specific Absorption Rate for Cancer Cell Hyperthermia Treatment. *ACS Nano* 6, 3080–3091 (2012).
2. Guardia, P. et al. One pot synthesis of monodisperse water soluble iron oxide nanocrystals with high values of the specific absorption rate. *J. Mater. Chem. B* 2, 4426 (2014).
3. Sathya, A. et al. Cox Fe<sub>3</sub>-xO<sub>4</sub> Nanocubes for Theranostic Applications: Effect of Cobalt Content and Particle Size. *Chem. Mater.* 28, 1769–1780 (2016).
4. Guardia, P. et al. Gold-iron oxide dimers for magnetic hyperthermia: the key role of chloride ions in the synthesis to boost the heating efficiency. *J. Mater. Chem. B* 5, 4587–4594 (2017).
5. Riedinger, A. et al. Post-Synthesis Incorporation of <sup>64</sup>Cu in CuS Nanocrystals to Radiolabel Photothermal Probes: A Feasible Approach for Clinics. *J. Am. Chem. Soc.* 137, 15145–15151 (2015).

## ACTIVITY REPORT

### *Research Activity*

#### *Research Period Abroad*

#### *Scientific Publications*

1. Najafshirtari, S.; Lak, A.; Guglieri, C.; Marras, S.; Brescia, R.; **Fiorito, S.**; Sadrollahi, E.; Litterst, F. J.; Pellegrino, T.; Manna, L.; Colombo, M. *RSC Adv.* 2018, 8 (40), 22411–22421.
2. Lak, A.; Cassani, M.; Mai, B. T.; Winckelmans, N.; Cabrera, D.; Sadrollahi, E.; Marras, S.; Remmer, H.; **Fiorito, S.**; Cremades-Jimeno, L.; et al. *Nano Lett.* 2018, 18, 6856–6866.

#### *Conferences attended:*

1. 15<sup>th</sup> International conference on Nanoscience & Nanotechnologies (NN18), 3 -6 July 2018, Thessaloniki, Greece

### *Courseware*

#### *Courses attended and passed:*

#### *Courses given by teachers of the Unige and IIT:*

1. Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations (1 CFU)
2. Basics of Crystallography and Diffraction by crystals (1 CFU)
3. Introductory course on transmission electron microscopy (1CFU)
4. Opto-Electronic Properties of Semiconductor Quantum Dots (1 CFU)
5. Spectroscopies for chemical analysis (1 CFU)
6. Mechanical properties + atomic force microscopy (1 CFU)
7. Water soluble nanoparticles (1 CFU)

8. Introductory on magnetism at the nanoscale (1 CFU)
9. Magnetic nanoparticles in nanomedicine (1 CFU)

***Courses given by invited experts:***

1. "An introduction to nanoscale magnetism for biomedical applications" Speaker: Neil Telling
2. "Approaches to synthesis and characterization of magnetic nanomaterials for biomedical applications", Speaker Davide Peddis
3. "From crystallography to imaging", Speaker: Cinzia Giannini

***Seminars attended:***

1. "Colloidal double quantum dots" Speaker: Dan Oron; 14<sup>th</sup> February 2017. Approaches to synthesis characterization of magnetic nanomaterials for biomedical applications
2. "From cancer biology to drug treatment: Oxaliplatin in the era of personalized medicine" Speaker: Paola Perego; 28<sup>th</sup> February 2017.
3. "Interplay of electronic and dynamical processes in organohalide Perovskites" Speaker: Filippo De Angelis; 14<sup>th</sup> March 2017.
4. "The future of monitoring serotonin (and other neurotransmitters) in Vivo" Speaker: Anne M. Andrews; 20<sup>th</sup> March 2017.
5. "Synthetic methodology for colloidal nanomaterials: limitations and opportunities" Speaker: Dmitri Talapin; 26<sup>th</sup> May 2017.
6. "High-throughput design of doped colloidal nanocrystals" Speaker: Emory Chan; 1<sup>st</sup> June 2017.
7. "Perovskite nanocrystals – the new generation of defect tolerant luminescent materials" Speaker: Sameer Sapra; 13<sup>th</sup> June 2017.
8. "Standardization methods for the synthesis of single-core and multi-core magnetic nanoparticles for medical applications", Speaker: Helena Gavilan Rubio; 2<sup>nd</sup> October 2017
9. "Aberration-corrected STEM: sub-Å resolution imaging, atomic-resolution elemental mapping, and vibrational spectroscopy", Speaker: Ondrej L. Krivanek; 4<sup>th</sup> October 2017
10. Synthesis of nanostructured stimuli-responsive materials for controlled drug delivery to treat cancer", Speaker: Hermis Iatro; 5<sup>th</sup> December 2017.
11. "Playing Lego at the nanoscale: Nanoparticles as building blocks for hierarchical structures", Speaker: Pablo Guardia; 11<sup>th</sup> December 2017.
12. "The physics of the Universe, over more than 60 orders of magnitude of length" Speaker: Antonio Ereditato; 18<sup>th</sup> December 2017.
13. "Design of magnetic nano-architecture for biomedical applications" Speaker: Davide Peddis; 24<sup>th</sup> January 2018.
14. "Nanobiosensors for diagnostics applications" Speaker: Arben Merkoçi; 31<sup>st</sup> May 2018.
15. "Engineering of Iron Oxide Nanoparticles for Magnetic Particle Imaging Guided-Hyperthermia (hMPI)" Speaker: Anna C. Samia; 6<sup>th</sup> June 2018.
16. "Probing magnetic properties of magnetic colloids or nanoparticles by AC magnetometry" Speaker: Francisco J. Teran, 18<sup>th</sup> January 2019.

***National and International Schools or Workshops:***

1. 12<sup>th</sup> International Summer schools "N&N: Organic Electronics & Nanomedicine" (ISSON18), 30 June-7 July 2018, Thessaloniki, Greece (3 CFU)
2. RADIOMAG cost action final meeting, 16-18 October 2018, Florence, Italy

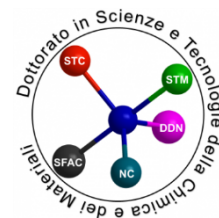


### ***Internal meetings***

1. Nanomaterials for Biomedical Applications annual group meeting, 7<sup>th</sup> June 2017, Italian Institute of Technology
2. Nanomaterials for Biomedical Applications annual group meeting, 19<sup>th</sup> July 2018, Italian Institute of Technology
3. Nanomaterials for Biomedical Applications annual group meeting, 17<sup>th</sup> June 2019, Italian Institute of Technology



Università degli Studi di Genova  
Doctorate in  
Sciences and Technologies of  
Chemistry and Materials



Curriculum: Pharmaceutical, Food and Cosmetic Sciences

VALERIA FRANCESCONI

**Start of the Doctorate Program:** November 1<sup>st</sup>, 2016  
**End of the Doctorate Program:** October 31<sup>st</sup>, 2019  
**Advisor:** Prof. Michele Tonetti

**Thesis Title:** Synthesis and biological evaluation of nitrogen heterocycle systems as potential antiviral agents.

**Thesis abstract**

Viruses are obligate intracellular parasites that consist of either double- or single-stranded DNA or RNA enclosed in a protein coat called capsid. Some viruses also possess a lipid envelope that, like the capsid, may contain antigenic glycoproteins. Most of them contain or encode enzymes essential for their replicative cycle inside host cells, sometimes usurping their metabolic machinery.

Traditional therapeutic approaches have mostly focused on targeting specific viral components or enzymes. This pathogen-directed strategy, while successful in numerous cases, in many others results ineffective due to the emergence of drug-resistance. A different approach, addressed to target host-factors essential for viral replication, has recently draw an increasing attention.

The principal activity of my Ph.D. thesis will be oriented to the synthesis of new nitrogen heterocycle systems as potential antivirals, directed in particular against RNA viruses belonging to *Flaviviridae*, *Orthomyxoviridae* and *Paramyxoviridae* families, including pathogens responsible for diseases with a high epidemiological impact, such as BVDV in cattle and HCV in humans, influenza A and B viruses and respiratory syncytial virus (RSV).

The project will be organized into the following phases:

1. Chemical synthesis of the novel compound series. The project is focused on the investigation of three different chemotypes, in order to obtain new antiviral agents: the acridine nucleus, the dihydrotriazine scaffold and the benzimidazole ring. Previous studies performed by the research group where I develop my Ph.D. thesis, revealed that all of these different classes of compound are endowed with an intrinsic antiviral activity; thus during my Ph.D. research work I will explore various possibilities of functionalisation of the three different scaffolds, with the aim of increasing their potency and selectivity profiles towards the respective antiviral target.
2. Characterization of the new compounds. Each newly synthesized compound will be characterised by spectroscopic methods (such as UV, IR, H-NMR and C-NMR) and elemental analysis.
3. Evaluation of cytotoxicity and antiviral activity in vitro. Against viruses belonging to *Flaviviridae*, *Orthomyxoviridae* and *Paramyxoviridae* families.

4. Evaluation of antiviral activity in vitro against other RNA and DNA viruses, to confirm selectivity.
5. Confirmation of the mechanism of action. The confirmation of the target will be supported by enzymatic assays and binding affinity assays.
6. SAR analysis, supported by computational studies.

# ACTIVITY REPORT

## Research Activity

### *Research Period Abroad*

Research period abroad (6 months) spent at the University of Barcelona (UB) in the Laboratory of Medicinal Chemistry, from the 11th June to the 31st of December 2018.

### *Scientific Publications*

1. Loddo, R., **Francesconi V.**, Laurini E., Boccardo S., Fermeglia, M., Pricl, S., Tonelli, M. "9-Aminoacridine- based agents impair the bovine viral diarrhea virus (BVDV) replication targeting the RNA-dependent RNA polymerase (RdRp)", *Bioorg. Med. Chem.*, 2018, 26(4), 855-868.
2. **Francesconi V.**, Giovannini L., Santucci M., Cichero E., Costi M.P., Naesens L., Giordanetto F., Tonelli M., "Synthesis, biological evaluation and molecular modeling of novel azaspiro dihydrotriazines as influenza virus inhibitors targeting the host factor dihydrofolate reductase (DHFR)", *Eur. J. Med. Chem.*, 2018, 155, 229-243.

### *Communications at Conferences*

#### *Oral communications:*

1. **Francesconi, V.**, Laurini, E., Pricl, S., Loddo, R., Tonelli, M., "9-Aminoacridine-based agents impair the Bovine Viral Diarrhea Virus (BVDV) replication targeting the RNA-polymerase (RdRp)". *La Giornata della Chimica Ligure*, Genova, October 20th, 2017.
2. **Francesconi, V.**, Laurini, E., Pricl, S., Loddo, R., Tonelli, M., "9-Aminoacridine-based agents impair the bovine viral diarrhea virus (BVDV) replication targeting the RNA-dependent RNA Polymerase (RdRp)". *MYCS - Merck Young Chemists Symposium*, Milano Marittima (Italy), November 13th-15th, 2017.

#### *Poster Communications:*

1. **Francesconi, V.**, Gazzarrini, S., Santucci, M., Cichero, E., Costi, M. P., Naesens, L., Tonelli, M. "Synthesis of 4,6-diamino-1,2- dihydrotriazines as influenza viruses and respiratory syncytial virus inhibitors targeting the host DHFR". "XXVI Congresso Nazionale della Società Chimica Italiana": *Conference Proceedings*, page 34. Paestum 10-14/09/2017.
2. **Francesconi, V.**, Giovannini, L., Cichero, E., Naesens L., Giordanetto, F., Tonelli M., "Development of novel azaspiro dihydrotriazines as influenza virus inhibitors targeting the host factor

- dihydrofolate reductase (DHFR)". XV Young Research Fellow Meeting – YRFM 2018, Orlèans, March 5th-7th, 2018; Book of Abstracts, P21.
3. **V. Francesconi**, E. Cichero, L. Naesens, M.P. Costi, M. Tonelli. Host DHFR-targeting (2-aminotriazino)benzimidazoles as new antiviral agents. XXVI Young Research Fellow Meeting – YRFM 2019, Paris (France), February 20th-22nd 2019, Book of Abstracts P61.
  4. **V. Francesconi**, L. Naesens, M. Tonelli. Synthesis and biological evaluation of novel (thio)semicarbazone-based benzimidazoles as antiviral agents. 6th-ECBS/LS-EuChemS 2019, Madrid (Spain), April 3rd-5th 2019, Book of Abstracts, pag 138.
  5. **V. Francesconi**. Synthesis of triazino derivatives as DHFR inhibitors for antiviral drug development. XXXIX ESMEC, Urbino, Palazzo Battiferri (Italy), June 30 - July 4, 2019, Book of Abstracts, P26.
  6. **V. Francesconi**, E. Cichero, L. Naesens, M.P. Costi, M. Tonelli. Development of new antifolates as host- based therapeutics to control influenza virus. XXVI National Meeting in Medicinal Chemistry, Milan, Ca' Granda, July 16-19, 2019, Book of Abstracts, P46.

### ***Congresses Attended***

1. La Giornata della Chimica Ligure, Genova (Italy), October 20th, 2017.
2. MYCS - Merck Young Chemists Symposium, Milano Marittima (Italy), November 13th-15th, 2017.
3. XV Young Research Fellow Meeting – YRFM 2018, Orlèans (France), March 5th-7th, 2018.
4. GIFC 2018, Giornate Italo-Francesi di Chimica, Genova (Italy), April 16th-18th, 2018.
5. XXVI Young Research Fellow Meeting – YRFM 2019, Paris (France), February 20th-22nd 2019.
6. 6th-ECBS/LS-EuChemS 2019, Madrid (Spain), April 3rd-5th 2019.  
XXVI National Meeting in Medicinal Chemistry, Milan, Ca' Granda, July 16th-19th, 2019.

## ***Courseware***

### ***Courses attended and passed***

#### ***B-type Courses Given by Teachers of the UNIGE and IIT:***

1. "INN and IUPAC nomenclature of organic drugs", Prof. Giancarlo Grossi (2 credits).
2. "Design and synthesis of protein-kinase inhibitors as anticancer agents", Prof. Silvia Schenone (2 credits).
3. "Instrumental techniques for trace elements determination in pharmaceuticals, food products and environmental samples", Prof. Minganti, Prof. Drava (2 credits).
4. "Patent and bibliographic databases searching in medicinal chemistry". Prof. Fossa, Prof. Brullo (2 credits).
5. "Molecular markers of food quality and genuineness", Prof. Boggia, Prof. Zunin (2 credits).

#### ***Courses Given by invited experts:***

1. "Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials; Novel Materials for energy storage and conversion" Prof. Dr. Thomas Fässler, University of Munich, Germany. Dipartimento di Chimica e Chimica Industriale, 11/05/2017.

2. "An introduction to nanoscale magnetism for biomedical applications", Dr. Neil Telling, Keele University, UK. IIT, 23-24/05/2017.
3. "Recent advances in computer-aided drug design", Prof. Tiziano Tuccinardi, University of Pisa, th Genova, October 16th, 2017.
4. "Probing Matter with Synchrotron Radiation", Dott. Luigi Paolasini (European Synchrotron Radiation Facility, Grenoble Cédex France) 28-29 May 2019 (DCCI).
5. "Organic Synthesis and Catalysis in the Pharmaceutical Industry", Dott. Paolo Tosatti (Senior Scientist, Roche, Basel), 20 september 2019 (DCCI).

### ***National and International Schools or Workshops***

1. ESMEC (37th Edition of the European School of Medicinal Chemistry) Urbino, 2-6/07/2017.
2. ESMEC (39th Edition of the European School of Medicinal Chemistry) Urbino, Palazzo Battiferri, 30/06/2019 -04/07/2017.
3. IV CADD-ISS Computer-Aided Drug Design International Summer School, Pisa, 8-13/07/2019.

### ***Seminars attended***

1. "Principi attivi (API) ed eccipienti: normativa, qualità e fabbricazione", Dr. Piero Iamartino, AFI. 11/11/2016
2. "Il marketing cosmetico: dalla mission aziendale alla risposta del consumatore", Dr.ssa Silvia Rum, Università degli Studi di Genova. 18/11/2016
3. "Odori, profumi e feromoni come mediatori chimici olfattivi", Dr.ssa Chiara Lacapra, Università degli Studi di Genova. 18/11/2016
4. "Giocare sporco: PAINS e composti promiscui", Dr.ssa Anita Parricchi, Università degli Studi di Genova. 18/11/2016
5. "Tubercolosi ed altre patologie polmonari", Dr.ssa Elda Meta, Università degli Studi di Genova. 18/11/2016
6. "Chemical biology and medicinal chemistry of human proteasomes", Prof. Herman Overkleeft, Leiden Institute of Chemistry. IIT, 20/12/2016
7. "I vaccini, dalle origini ai giorni nostri", Dott.ssa Sanna Monica, University of Genova. October 18th, 2017.
8. "Chronic Obstructive Pulmonary Disease (COPD): a pathology overview and the possible effects of Particulate Matter (PM)", Dott. Brignole Daniele, University of Genova. October 18th, 2017.
9. "Imaging in Oncology" Dott.ssa Pastorino Sara, University of Genova. October 18th, 2017.
10. "Depressione e nuove strategie terapeutiche", Dott. Sadeghi Mohamed, University of Genova. October 18th, 2017.
11. "Probiotics: properties, uses and interaction with human gut microbiome", Dott.ssa Turrini Federica, University of Genova. October 18th, 2017.
12. "Il controverso ruolo della beta-amiloide nella malattia di Alzheimer", Roberta Ricciarelli, 30 January 2019 DIMES, Anatomia Umana.
13. "Screening of mixed co-poly(ester-carbonate) PEG-based nanoparticles for breast cancer therapy: an in vitro and biodistribution based approach", Dr Robert Cavanagh (University of Nottingham) 26th March 2019 (DIFAR).
14. "Using polymer 3D architecture, size and chemistry to control nanoparticle distribution for Doxorubicin drug delivery in vitro and in vivo", Dr Amanda Pearce (University of Birmingham) 26th March 2019 (DIFAR).

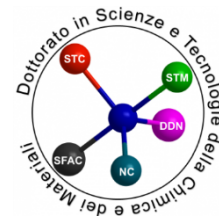
15. "Organocatalysed synthesis and characterization of a small library functionalisable co-poly(ester)-(carbonate)s initiated by varying pegylated architectures and labile-(meth)acrylate esters" by Dr Vincenzo Taresco (University of Nottingham) 26<sup>th</sup> March 2019 (DIFAR).
16. "Preliminary in vitro assays to evaluate anticancer drugs", Dott.ssa Chiara Greco, Università di Genova, 15/10/2019, DIFAR.
17. "Design of Experiment: Full Factorial Design and Case Study" Dott.ssa Maryam Hooshyari, Università di Genova, 15/10/2019, DIFAR.
18. "Combination of conventional antibiotics with natural products: a promising strategy in overcoming antibiotic resistance", Dott.ssa Francesca Pedrelli, Università di Genova, 15/10/2019, DIFAR.
19. "Production of biopharmaceutical proteins: particular case of the plants" Dr. Dougué Kentsop Roméo Arago, Università di Genova, 15/10/2019, DIFAR.

### ***Other Activities***

1. Speaker of a seminar held within the Doctoral School of Chemical and Materials Sciences and Technologies titled: "Astrochemistry: the chemistry of stars" Dr.ssa Valeria Francesconi, Università degli Studi di Genova (DIFAR), 15/10/2019



**Università degli Studi di Genova**  
**Doctorate in**  
**Sciences and Technologies of**  
**Chemistry and Materials**



**Curriculum: Nanochemistry**

**SILVIA GENTILUOMO**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*

**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*

**Advisors:** Dr. Francesco Bonaccorso (IIT), Dr. Vittorio Pellegrini (IIT),  
Prof. Daniele Marrè (UniGe)

**Thesis Title:** Science and technology of graphene-based inks for polymer-composite applications

**Thesis abstract**

Graphene is exploited in the polymer composites field as filler, due to its capacity to improve the properties of the polymer matrix. However, it is important to use scalable methods, both for the production of graphene and the preparation and manufacturing of the graphene-polymer composites. In this study, graphene is produced through wet jet milling (WJM), a technique based on the exfoliation of graphite by high shear rate, which allows to produce graphene dispersions<sup>1</sup> with a concentration up to 3 g L. The graphene-polymer composites are prepared by using styrene-butadiene copolymer (SB) as matrix and melt mixing the graphene and SB powder by means of extrusion. Subsequently, two different manufacturing techniques are used to prepare the samples, compression and injection molding. The effect of the manufacturing techniques on the mechanical and thermal properties of the composites is studied. The injection molded samples (IM) give the best results in terms of mechanical properties, reaching an improvement of 60 % and 30 %, with respect to the pristine SB polymer, for the Young's modulus and the tensile strength, respectively, by using 15 wt % of graphene flakes. Instead, the compression molded samples (CM) show a higher thermal conductivity than the IM samples, achieving an enhancement of 170 % compared with the bare matrix, still with 15 wt % of loading.

# ACTIVITY REPORT

## *Research Activity*

### *Scientific Publications*

1. **S. Gentiluomo**<sup>#</sup> et al., “Fire behavior of polyamide 12 nanocomposites containing POSS and CNT”, *Polym. Degrad. Stab.*, 134 (2016)151-156
2. E. Petroni, E. Lago, S. Bellani, D.W. Boukhalov, A. Politano, B. Gürbulak, S. Duman, M. Prato, **S. Gentiluomo**, R. Oropeza-Nuñez, J.K. Panda, P.S. Toth, A.E. Del Rio Castillo, V. Pellegrini, and F. Bonaccorso, “Liquid-Phase Exfoliated Indium–Selenide Flakes and Their Application in Hydrogen Evolution Reaction”, *Small* 14 (2018) 1800749
3. A.E. Del Rio Castillo, A. Ansaldo, F. Ricciardella, H. Sun, L. Marasco, J. Buha, Z. Dang, L. Gagliani, **S. Gentiluomo**, E. Lago, P. Toth, N. Curreli, F. Palazon, A. Tomadin, M. Polini, V. Pellegrini, and F. Bonaccorso, “High yield production of 2D crystals by wet-jet milling”, *Mater. Horiz.* (2018), Advance Article, DOI: 10.1039/C8MH00487K
4. E. Lago, F. Bonaccorso, **S. Gentiluomo**, A.E. Del Rio Castillo, N.M. Pugno, R. Cingolani, P.S. Toth, and V. Pellegrini, “Exploiting the ideal properties of two-dimensional fillers for the mechanical reinforcement of polymer nanocomposites”, submitted
5. **S. Gentiluomo**<sup>#</sup> et al., “Graphene production and enhancement of its ABS composite properties”, work in progress and
6. S.B. Thorat<sup>#</sup>, **S. Gentiluomo**<sup>#</sup>, E. Lago, P.S. Toth, N. Curreli, U. Paul, A. Athanassiou, V. Pellegrini, and F. Bonaccorso, “Exfoliation of boron nitride in water-surfactant medium and their influence on the poly-lactic acid composites to enhance the mechanical and gas barrier properties”, work in progress
7. **S. Gentiluomo**<sup>#</sup> et al., “Study of mechanical, thermal and tribological properties of 3D printed graphene- polyamide 6 composites”, work in progress
8. **S. Gentiluomo**<sup>#</sup> et al., “Effect of processing on the mechanical and thermal properties of graphene based styrene-butadiene-styrene copolymer composites”, work in progress

### *Oral contributions*

1. **S. Gentiluomo**, S. B. Thorat, E. A. Del Rio Castillo, V. Pellegrini, and F. Bonaccorso, “Poly methyl methacrylate assisted exfoliation of graphite and its use in acrylonitrile butadiene styrene composites”, *Nanotextology*, Thessaloniki (Greece), 29/06/2019 – 06/07/2019
2. S. B. Thorat, A. E. Del Rio Castillo, S. Natalini, E. Lago, **S. Gentiluomo**, L. Marasco, S. Bortolotti, J. K. Panda, R. Oropeza, V. Pellegrini and F. Bonaccorso, “Graphene polymer composites: the effect of flakes aspect ratios on the composite properties”, *Graphene week*, San Sebastian (Spain), 10/09/2018-14/09/2018
3. **S. Gentiluomo**, P. S. Toth, E. Lago, S. B. Thorat, V. Pellegrini, and F. Bonaccorso, “Use of poly (methyl methacrylate) for the graphene and polymer composites production”, *Graphene 2018*, Dresden (Germany), 26/06/2018 – 29/06/2018



4. E. Lago, P.S. Toth, **S. Gentiluomo**, S.B. Thorat, V. Pellegrini and F. Bonaccorso, “Unravelling the boron nitride flakes morphology to enhance polycarbonate performances”, Imaginenano 2018, GraphIn, Bilbao (Spain), 13/03/2018 – 15/03/2018
5. **S. Gentiluomo**, P.S. Toth, E. Lago, S.B. Thorat, M. Prato, V. Pellegrini and F. Bonaccorso, “Application of functional polymer inks: two-dimensional crystals production and enhancement of their polymer composites properties”, MRS 2017 Fall Meeting, Boston (USA), 26/11/2017 - 01/12/2017 MRS 2017 Fall Meeting, Boston (USA), 26/11/2017 - 01/12/2017
6. Del Rio Castillo, A. Ansaldo, F. Ricciardella, Hayan Sun, **S. Gentiluomo**, V. Pellegrini, and F. Bonaccorso, “Gram scale production of large size 2D crystals”, MRS 2017 Fall Meeting, Boston (USA), 26/11/2017 - 01/12/2017
7. E. Del Rio Castillo, A. Ansaldo, F. Ricciardella, H. Sun, **S. Gentiluomo**, S. Enriquez, V. Pellegrini, and F. Bonaccorso, “Large scale production of 2D crystals by wet jet milling” Materials.it, Catania (Italy), 12/12/2016–16/12/2016
8. **S. Gentiluomo**, P. S. Toth, V. Pellegrini, and F. Bonaccorso “Exfoliation of graphite in green solvents: Scalable graphene production for polymer composites”, Materials.it, Catania (Italy), 12/12/2016 – 16/12/2016
9. Ansaldo, A. E. Del Rio Castillo, F. Ricciardella, **S. Gentiluomo**, V. Pellegrini, and F. Bonaccorso, “High yield production of large size few layer 2D crystals dispersions by wet jet milling”, Graphene 2016, Genova (Italy), 19/04/2016-22/04/2016

#### ***Poster contributions***

1. E. Lago, P.S. Toth, **S. Gentiluomo**, S.B. Thorat, V. Pellegrini and F. Bonaccorso, “Unravelling the boron nitride flakes morphology to enhance polycarbonate performances”, MRS 2017 Fall Meeting, Boston (USA), 26/11/2017 - 01/12/2017
2. E. Lago, P.S. Toth, **S. Gentiluomo**, S.B. Thorat, V. Pellegrini and F. Bonaccorso, “Unravelling the boron nitride flakes morphology to enhance polycarbonate performances”, Graphene 2017, Barcelona (Spain), 28/03/2017 – 31/03/2017
3. E. Lago, P.S. Toth, **S. Gentiluomo**, S.B. Thorat, V. Pellegrini and F. Bonaccorso, “Enhancing polycarbonate performances by adding environmentally friendly liquid-phase exfoliated boron nitride flakes” Materials.it, Catania (Italy), 12/12/2016 – 16/12/2016

#### ***International schools***

1. Summer school: “Bayreuth International Summer School (BISS) 2018”, 01/07/2018 – 14/07/2018, 3 ECTS (3-4 CFU)

## ***Courseware***

#### ***Courses attended and passed***

#### ***Courses given by teachers of the Unige and IIT:***

1. Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations (1 CFU)
2. Basics of Crystallography and Diffraction by crystals (1 CFU)
3. Introductory course on transmission electron microscopy (1 CFU)

4. Characterization of polymeric materials (6 CFU)
5. Mechanical properties + atomic force microscopy (1 CFU)
6. Spectroscopies for chemical analysis (1 CFU)
7. Introduction to functional ceramic materials: structure, properties, preparation and applications (2 CFU)
8. Optical Spectroscopy of Colloidal Nanocrystals (1 CFU)

### ***A-type courses giveb by invited experts***

1. Basics in Electrochemistry (1 CFU)
2. Spectroscopies for chemical analysis (1 CFU)
3. Chemistry and Physics of "Materials Science of Borides and particularly of Metal Boron Carbides (1 CFU)
4. From cristallography to Imaging (1 CFU)

### ***Seminars***

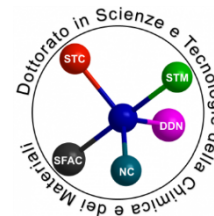
1. "From chemical complexity to functional complexity: tailoring multifunctional low dimensional materials and devices", P. Samorì, 14/11/2016
2. "The Electrochemical & Physical Performance Benefits of Graphene into Li-ion Energy Storage Technologies", M. Loveridge, 15/09/2017
3. "Mesoscopic thermodynamics", K. Ensslin, 07/02/2017
4. "Graphene-based membranes", S. Garaj, 11/03/2017
5. "Van der Waals assembly of 2D materials for devices applications", G. H. Lee, 16/01/2017
6. "The physics of the Universe, over more than 60 orders of magnitude of length", A. Ereditato, 18/12/2017
7. "Graphene and other 2D related materials interface engineering for highly efficient and stable organic and perovskite solar cells", E. Kymakis, 14/11/2017
8. "The new generation of energy storage devices: sulfur, lithium metal and nonflammable electrolytes", L. Carbone, 16/02/2018
9. "Membrane engineering", E. Drioli, 05/02/2018
10. "Quantum optics of two-dimensional materials: from many-body physics to quantum information", G. Grosso, 17/04/2018
11. "One-year stable perovskite solar cells by 2D/3D interface engineering", G. Grancini, 02/02/2018
12. "LiFe<sub>1-x</sub>YMnxCoyPO<sub>4</sub> olivine materials in novel lithium-ion and lithium –metal cells", D. Di Lecce, 30/08/2018
13. "A special road of bringing consumer robots to the world – UBTECH Robotics Corp", J. Pang, 06/09/201
14. "Publishing in Nature nanotechnology" – C. Pastore, 27/09/201815)
15. "Graphene materials in thermoplastics. Preparation, applications and potential markets", J.G. Cordon, 06/12/2018 16) "Future applications for graphene: the printing of immune cells", L. G. Delogu, 04/03/2019
16. "Novel plasmonic and photonic nanomaterials for optoelectronic and bio applications", G. Tselikov, 04/03/2019

## ***Collaborations***

Collaboration with Foundation for Research and Technology (FORTH), Hellas, Greece, 31/03/2019–27/06/2019



Università degli Studi di Genova  
Doctorate in  
Sciences and Technologies of  
Chemistry and Materials



Curriculum: Pharmaceutical, Food and Cosmetic Sciences

CHIARA GRECO

**Start of the Doctorate Program:** November 1<sup>st</sup>, 2016

**End of the Doctorate Program:** October 31<sup>st</sup>, 2019

**Advisor:** Prof.ssa Sivia Schenone

**Thesis Title:** Synthesis and biological evaluation of pyrazolo[3,4-*d*]pyrimidine derivatives active as SGK1, Fyn and Src kinases inhibitors

**Thesis abstract**

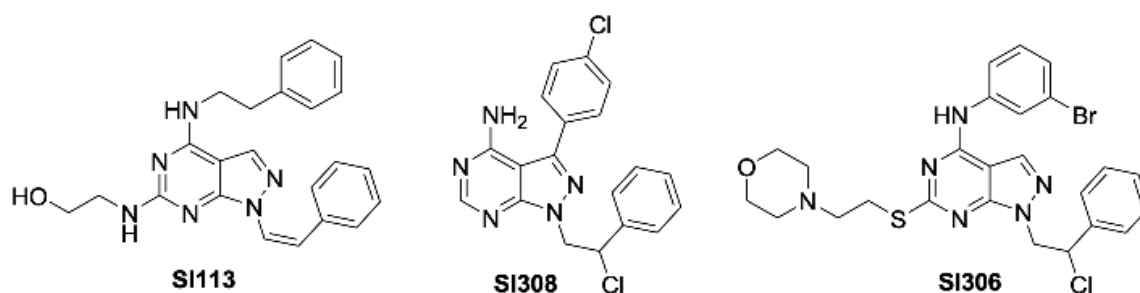
The pathogenesis of many cancers is characterized by mutations, overexpression and dysregulation of protein kinases. As a result, increasing attention has been directed towards the identification of novel kinase inhibitors for cancer therapy<sup>1</sup>. The work performed here focuses on the synthesis of a series of pyrazolo[3,4-*d*]pyrimidine derivatives as inhibitors of the serine-threonine kinase SGK1, and the tyrosine kinases Fyn and Src.

The first set of compounds are analogues of the in house SGK1 inhibitor SI113 (**Fig.1**) which had previously demonstrated anti-cancer activity. In fact SI113 resulted to be active on various cancer cell lines and in an *in vivo* hepatocellular carcinoma model<sup>2</sup>. The new set of SI113 analogues are characterized by different anilines, amines and a morpholine group in C4 and are decorated in C6 with polar chains, i.e. ethanolamine, diethanolamine, ethylene glycol and ethylenediamine. The double bond on the N1 side chain which is essential for the activity of compounds toward SGK1, was maintained.

The structures of the second set of compounds, instead, are related to the in house Fyn inhibitor SI308 (**Fig.1**). From previously studies on the first generation of Fyn inhibitors, SI308 was reported as the most potent compound, demonstrating both antiproliferative activity on cancer cell lines and the ability to inhibit protein 3Tau phosphorylation in a cellular model of Alzheimer's disease<sup>3</sup>. The new generation of SI308 related compounds present a methyl group at the C6 position and on C3 the phenyl ring is either unsubstituted or presents a methyl group in para position. Preliminary screening using enzyme activity assays demonstrates that some of the novel compounds are active and therefore suitable for further study using *in vitro* models. It is predicted that subsequent *in vitro* data will aid in the design of future compounds.

Furthermore, previous data on another in house compound SI306 (**Fig.1**), which is active on tyrosine kinase Src, reported promising results on an *in vivo* xenograft model of neuroblastoma<sup>4</sup>. To further study this biological activity, SI306 was re-synthesized and additional experiments were performed on *in vitro* models. Testing of this compound on MYCN-amplified neuroblastoma cell lines HTLA-230 and SK-N-BE-2C further confirmed the activity of SI306 and provide increased support for the inhibition of Src as a valid approach for neuroblastoma treatment.

Finally, further *in vitro* studies were performed on of the three previously cited in house pyrazolo[3,4-*d*]pyrimidines, SI306, SI308 and SI113, using patient derived glioblastoma multiforme (GBM) cell lines. This final set of work was undertaken during a visiting research fellowship period and performed in collaboration with the School of Pharmacy at the University of Nottingham (United Kingdom). Kinase inhibitor activity has been evaluated on series of patient derived GBM cell lines isolated from both the central tumor core (GCE28) 5 and from the invasive margin of the tumor (GIN28 and GIN8)<sup>5</sup>. The use of such phenotypically relevant *in vitro* models represents an important step for GBM drug development and screening. The results gathered using these relevant cell models further demonstrate the anti-cancer activity of the pyrazolo[3,4-*d*]pyrimidines compounds. Moreover, investigating the compounds in combination with one another reveals that synergy can be achieved and this finding has additional implications for potentially overcoming GBM drug resistance. Additionally, to overcome the low water solubility of our pyrazolo[3,4-*d*]pyrimidines compounds, formulations of the lead compounds (SI306, SI308 and SI113) were prepared using miniaturized screening process based on inkjet printing technology<sup>6</sup>. The observed activity of our compounds *in vitro* taken together with their successful formulation highlight that our kinase inhibitors are attractive candidates for the treatment of GBM.



**Fig.1.** Structure of the in house pyrazolo[3,4-*d*]pyrimidines SI113, SI308, SI306.

#### REFERENCES

- Carles, F. *et al* *Molecules* **23**, 1–18 (2018).  
 Talarico, C. *et al.* *Oncotarget* **7**, 15868–15884 (2016).  
 Tintori, C. *et al.* *J. Med. Chem.* **58**, 4590–4609 (2015).  
 Tintori, C. *et al.* *J. Med. Chem.* **58**, 347–361 (2015).  
 Smith, S. J. *et al.* *Int. J. Mol. Sci.* **18**, (2017).  
 Sanna, M. *et al.* *ACS Med. Chem. Lett.* **9**, 193–197 (2018).

# ACTIVITY REPORT

## Research Activity

### **Research Period Abroad**

Visiting research fellowship in Nottingham University, Boots Science Building, Prof. Cameron Alexander (From 30<sup>th</sup> May 2018 until 2<sup>nd</sup> February 2019).

Work focused on the mode of action of new kinase inhibitors in a range of cell lines derived from the invasive margins of glioblastoma patients and evaluation of the compounds activity in some polymer therapeutic carriers.

### **Scientific Publications**

1. "Pyrrolo[2,3-d]pyrimidines active as Btk inhibitors", Musumeci F, Sanna S, **Greco C**, Giacchello I, Fallacara AL, Amato R, Schenone S. *Expert Opin Ther Pat.* 2017 Dec;27(12):1305-1318.
2. "An Update on JAK Inhibitors" Musumeci F, **Greco C**, Giacchello I, Fallacara AL, Ibrahim MM, Grossi G, Brullo C, Schenone S. *Curr Med Chem.* 2018;26(10):1806-1832.
3. "Recent Studies on Ponatinib in Cancers Other Than Chronic Myeloid Leukemia", Musumeci F, **Greco C**, Grossi G, Molinari A, Schenone S. *Cancers.* 2018 Nov 9;10(11).
4. "Identification of a new family of pyrazolo[3,4-d]pyrimidine derivatives as multitarget FynBlk-Lyn inhibitors active on B- and T-lymphoma cell lines", Fallacara AL, Passannanti R, Mori M, Iovenitti G, Musumeci F, **Greco C**, Crespan E, Kissova M, Maga G, Tarantelli C, Spriano F, Gaudio E, Bertoni F, Botta M, Schenone S. *Eur J Med Chem.* 2019 Jul 18;181:111545.
5. "Insights into RNA-dependent RNA Polymerase Inhibitors as Anti-influenza Virus Agents", Giacchello I, Musumeci M, D'Agostino I, **Greco C**, Grossi G and Schenone S. Submitted to *Current Medicinal Chemistry*:

### **Communications at Conferences**

#### **Poster communications:**

1. "Synthesis of a new generation of pyrazolo[3,4-d]pyrimidines as SGK-1 inhibitors", **Greco C**, Sanna M, Musumeci F, Giacchello I, Perrotti N, Alcaro S, Ortuso F, Schenone S. HSMC-2017 Aristotele University, Thessaloniki 1-3 June 2017. (3th place for BestPoster Award).
2. "Synthesis of a small library of potential SGK-1 inhibitors", **Greco C**, Musumeci F, Giacchello I, Perrotti N, Alcaro S, Ortuso F, Schenone S. GIFC-2018: Giornate Italo-Francesi di Chimica. April 16th – 18th 2018. Genova.
3. "Pyrazolo[3,4-d]pyrimidine active on neuroblastoma cells", **Greco C**, Musumeci F, Giacchello I, Gorjòn de Pablo G, Molinari A, Fallacara AL, Di Maria S, Botta M, Schenone S. VII EWDSy: European Workshop Drug Synthesis. May 20th-24th 2018. Siena.
4. "Formulated pyrazolo[3,4-d]pyrimidines active on GBM cell lines", **Greco C**, Cavanagh C, Taresco V, Petromilo H, Musumeci F, Rahman R, Alexander C, Schenone S. XII EWDD: 12th European Workshop in Drug Design. May 19th-24th 2019. Siena.

5. "Formulation Of Pyrazolo[3,4-d]pyrimidines Kinase Inhibitors For The Treatment Of Glioblastoma Multiforme", **Greco C**, Cavanagh C, Pearce A, Taresco V, Musumeci F, Rahman R, Alexander C, Schenone S. Controlled release society annual meeting and exposition. 20th-24th July 2019. Valencia, Spain.

### ***Congresses Attended***

1. 7th Hellenic Symposium on Medicinal Chemistry, HSMC-2017. June 1st -3rd 2017, Aristotele University, Thessaloniki (Greece)
2. Giornata della Chimica Ligure, October 20th 2017, Genova.
3. GIFC-2018: Giornate Italo-Francesi di Chimica, April 16th – 18th 2018. Genova.
4. 4th Annual Nanopharmaceutics Symposium. June 29th 2018, Keele (UK).
5. Controlled release society annual meeting and exposition, 20th-24th July 2019, Valencia, Spain.

## ***Courseware***

### ***Courses attended and passed***

#### ***Courses Given by Teachers of the Unige and IIT:***

1. "Design and synthesis of protein-kinase inhibitors as anticancer agents" Prof. Silvia Schenone. (2 credits).
2. "INN and IUPAC nomenclature of organic drugs" Prof. Giancarlo Grossi (2 credits).
3. "Molecular markers of food quality and genuineness" Professors Roberta Boggia and Paola Zunin (2 credits)
4. "Patent and bibliographic databases searching in medicinal chemistry" Professors Paola Fossa and Chiara Brullo (2 credits)
5. "Pharmaceutical Biotechnology" Prof. Mauro Mazzei (3 credits)

#### ***Courses Given by invited experts:***

1. "Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials" and "Novel Materials for energy storage and conversion", Prof. Dr. Thomas Fässler. May 11th 2017.
2. "Recent advances in computer-aided drug design", Prof. Tiziano Truccinardi. October 16th 2017.
3. "Organic Synthesis and Catalysis in the Pharmaceutical Industry", Dott. Paolo Tosatti, September 20<sup>th</sup> 2019.

### ***National and International Schools or Workshops***

1. Workshop di Federchimica: "Programma PhD: La formazione post lauream e il mondo del lavoro - Nell'Industria Chimica, chi fa Ricerca... fa Carriera?", July 25th 2017, Genova.
2. European School of Medicinal Chemistry (ESMEC), July 2-6 2017. Urbino.
3. VII EWDSy: European Workshop Drug Synthesis, May 20th-24th 2018, Siena.
4. XII EWDD:12th European Workshop in Drug Design, May 19th-24th 2019, Siena.

### ***Seminars attended:***

1. "Un caso di proficua collaborazione: biocatalisi e prodotti naturali", Dr. Sergio Riva. 12/06/2017

2. "Chemical biology and medicinal chemistry of human proteasomes", Prof. Herman Overkleeft. 20/12/2016
3. "Chronic Obstructive Pulmonary Disease (COPD): a pathology overview and the possible effects of Particulate Matter (PM)", Brignole Daniele, 18/10/2017 - "Imaging in Oncology", Pastorino Sara. 18/10/2017
4. "Depression: new therapeutic strategies", Sadeghi Mohamed. 18/10/2017, "The vaccines: from the origins to the present day", Sanna Monica, 18/10/2017
5. "Probiotics: properties, uses and interaction with human gut microbiome", Turrini Federica. 18/10/2017
6. "Screening of mixed co-poly(ester-carbonate) PEG-based nanoparticles for breast cancer therapy: an in vitro and biodistribution based approach", Dr Robert Cavanagh. 26/03/2019
7. "Using polymer 3D architecture, size and chemistry to control nanoparticle distribution for Doxorubicin drug delivery in vitro and in vivo", Dr Amanda Pearce. 26/03/2019
8. "Organocatalysed synthesis and characterization of a small library functionalisable co-poly(ester)-(carbonate)s initiated by varying pegylated architectures and labile- (meth)acrylate esters", Dr Vincenzo Taresco. 26/03/2019
9. "Lavorare tra normative e regolamenti nell'industria chimica: il Regulatory Affairs Manager" Federchimica, 12/04/2019
10. "Novel [18F] Fluorinated Radiotracers for PET Imaging", Prof. Matteo Zanda, 11/10/2019
11. "Astrochemistry: The chemist of stars", Valeria Francesconi, 15/10/2019
12. "Design of experiment. Full factorial design and case study", Maryam Hooshyari, 15/10/2019
13. "Combination of conventional antibiotics with natural products: a promising strategy in overcoming antibiotic resistance", Francesca Pedrelli, 15/10/2019
14. "Production of biopharmaceutical proteins: particular case of plants", Dougué Kentsop Roméo Arago, 15/10/2019
15. "Il paradigma multi-target nel riposizionamento e nella scoperta di sostanze biologicamente attive", Prof. Alcaro Stefano, 17/10/2019

### **Other Activities**

1. *Speaker of a seminar held within the Doctor School of Chemical and Material Sciences and Technologies titled: "Preliminary in vitro assays to evaluate anticancer drugs".*, 15/10/2019, DIFAR, University of Genoa.
2. *Tutor at University of Genoa:* Tutoring to Pharmacy students for preparing their oral and written exams regarding Biology and General Chemistry, October 2017- July 2019.
3. *Laboratory assistant at University of Genoa:* Demonstration and assistance for laboratory exercises for Pharmacy students; Ensuring laboratory safety; October 2017 – May 2019.





**Università degli Studi di Genova**  
**Doctorate in**  
**Sciences and Technologies of**  
**Chemistry and Materials**

**Curriculum: Drug Discovery and Nanobiotechnologies**

**MELISSA GUARDIGNI**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*

**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*

**Advisors:** Dr. Tiziano Bandiera (IIT), Dr. Fabio Bertozzi (IIT), Paola Fossa (UniGe)

**Thesis Title:** Design and synthesis of novel Cystic Fibrosis (CF) modulators – Development of novel inhibitors of the anti-infective target DXS using Dynamic Combinatorial Chemistry (DCC)

**Thesis abstract:**

**Part 1: Design and synthesis of novel Cystic Fibrosis (CF) modulators (IIT, Genova – IT)**

Cystic fibrosis is a lethal, autosomal recessive genetic disease characterized by an accumulation of viscous mucus at epithelia surface of multiple organs including the lungs, pancreas, gut and testes, which results in obstruction, infection, inflammation and ultimately organ failure. The fundamental cause of CF is the mutation of a gene, the cystic fibrosis transmembrane conductance regulator (CFTR), which cause a decrease in CFTR chloride channel function and a resulting lack of ionic and water homeostasis at epithelial surfaces. The lack of CFTR-dependent water homeostasis explains mucus viscosity elevation in these affected organs. Historically, conventional CF treatments has focuses on symptomatic therapy but nowadays, the growing understanding of the molecular basis of CF pathologies has stimulates the development of small-molecule drugs called CFTR modulators which address the primary cause of CF with the hope to repair the defects in CFTR. The aim of my PhD project will be focused on the design, synthesis and biological characterization of novel CFTR modulators.

**Part 2: Development of novel inhibitors of the anti-infective target DXS using Dynamic Combinatorial Chemistry (DCC) (HIPS, Saarbrücken – DE, Supervisor: Prof. Dr Anna K. H. Hirsch)**

Discovery and development of new antibiotic agents with novel targets and mechanisms of action are urgently needed due to the increase of antibiotic resistance developed by pathogen agents. The aims of this study is the development of selective and potent inhibitors of the important and underexplored anti-infective target DXS. This one is the first enzyme of the non-mevalonate (MEP) pathway which is absent in humans but is essential for medically relevant pathogens (e.g., *Plasmodium falciparum*, *Mycobacterium tuberculosis*, *Pseudomonas aeruginosa*, and methicillin-resistant *Staphylococcus aureus*) which uses this pathway for the biosynthesis of isoprenoid precursors, vitamins B1 and B6. To address these issues, we are using a combination of structure-based drug design and target-directed dynamic combinatorial

chemistry (tdDCC) as hit-identification strategies for the first time for DXS. To expand the structural diversity and obtain potent and selective inhibitors of DXS, we designed the dynamic combinatorial library for acyl hydrazone formation. Different heterocyclic hydrazides and aldehydes were chosen based on calculated estimated affinity using SeeSAR for all possible acyl hydrazone products. Biochemical evaluation of several hit compounds amplified in the tdDCC experiment against *M. tuberculosis* DXS and *D. radioduran* DXS afforded inhibitors with IC<sub>50</sub> in the range of 30 – 190 μM.

## ACTIVITY REPORT

### *Research Activity*

**Research Period Abroad:** at Helmholtz Institute for Pharmaceutical Research Saarland (HIPS) Saarbrücken – Germany, from 14/01/2019 to 12/07/2019; Project: Development of novel inhibitors of the anti-infective target DXS using Dynamic Combinatorial Chemistry (DCC) Supervisor: Prof. Dr Anna K. H. Hirsch

### *Congresses Attended*

1. “15th Convention of FFC investigators in cystic fibrosis” 11/2017, Verona.
2. “16th Convention of FFC investigators in cystic fibrosis” 11/2018, Verona.
3. “HIPS Symposium 2019”, June 27-28, 2019, , Saarbrücken – DE.

### *Courseware*

#### *B-type courses attended and passed*

#### *Courses Given by Teachers of the Unige and IIT*

1. Design and synthesis of protein-kinase inhibitors as anticancer agents. Prof. S. Schenone (UNIGE) (2 CFU)
2. D3 PhD courses (3 CFU):
  - Introduction to course – Dr. Angelo Reggiani
  - Target identification and validation- Dr. Benedetto Grimaldi
  - Hit identification compound collection and natural sources- Dr. Fabio Bertozzi
  - Hit to lead and lead optimization: medicinal chemistry, synthesis of drugs- Prof Renata Riva
  - Hit to lead and lead optimization: Chiral drug- Dr. Fabio Bertozzi
  - Hit to lead and lead optimization: Bioisosterism- Dr. Rita Scarpelli
  - Hit to lead and lead optimization: Improving drug likeness- Dr. Tiziano Bandiera
  - Hit to lead and lead optimization: Pharmacology- Dr Rosalia Bertorelli
  - Hit to lead and lead optimization: Pharmacology- Dr Angelo Reggiani
  - Patents- Dr Lorenzo Rossi and Dr. Giuseppe Giardina
3. Pharmaceutical Biotechnology. Prof. Mazzei (UNIGE) (3CFU);

4. Patent and bibliographic databases searching in medicinal chemistry. Prof. Fossa and Brullo (2 CFU);
5. Instrumental techniques for trace elements determination in pharmaceuticals, food products and environmental samples, Prof Minganti and Drava (2 CFU)
6. Perspectives on bioinorganic chemistry, Prof. S. De Negri (UNIGE) (2 CFU)

#### ***Type A Courses given by experts***

1. "Principles of Computer-aided Drug Design", Prof. Tiziano Tuccinardi (Università di Pisa e Sbarro Institute for Cancer Research and Molecular Medicine Center for Biotechnology, Temple University, Philadelphia), DIFAR 22/10/2018
2. Hit to Lead and Lead Optimization 07/07/2017: "Medicinal Chemistry" and "Improving drug-likeness", Dr. Tiziano Bandiera e "Bioisosterism", Dr. Rita Scarpelli
3. "Organic Synthesis and Catalysis in the Pharmaceutical Industry", Dr. Paolo Tosatti, (Senior Scientist, Roche, Basel), Genova DCCI, 20/02/2019
4. Concepts of Drug Discovery and Personalised Medicine 16/09/2019: "How to translate an idea into a drug discovery project: scientific and economical aspects" Dr Angelo Reggiani e "Introduction to pharmacokinetics and targeted nanomedicine", Dr Nicola Tirelli.
5. Concepts of Drug Discovery and Personalised Medicine, 01/10/2019: "From Hit Identification to Lead Optimization a medicinal chemistry overview", Dr Tiziano Bandiera e "Selectivity and specificity in drug discovery" Dr. Benedetto Grimaldi.
6. Concepts of Drug Discovery and Personalised Medicine, 17/09/2019 e 02/10/2019: "Paths to drug discovery and the role of computational chemistry" Dr. Marco De Vivo e "How to transform an experimental compound into a medicine" Dr. Angelo Reggiani.

#### ***National and International Schools or Workshops***

1. XLII International Summer School on Organic Synthesis "A. Corbella" ISOS 2017
2. European School of Medicinal Chemistry ESMEC" 2018, Urbino.

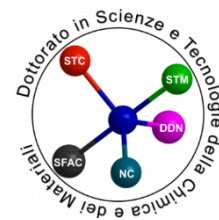
#### ***Seminars:***

1. "A cross-talk between lysosome and nucleus controls cell metabolism", Prof. Andrea Ballabio, Telethon Institute of Genetics and Medicine (TIGEM), Naples, Italy. April 5<sup>th</sup>, 2017
2. "Synthetic small-molecule RNA ligands: scope and applications", Dr. Maria Duca, Université Côte d'Azur, Institut de Chimie de Nice; 05/06/2018, (IIT)
3. "Spectroscopies for Chemical Analysis: introduction to NMR" Dr. Luca Goldoni, Istituto Italiano di Tecnologia, Genova, Italy; 12/06/2018, (IIT)
4. Protein Structure and Fragment-Based Drug Discovery in Cancer & Tuberculosis", Professor Sir Thomas L. Blundell - Department of Biochemistry, University of Cambridge; 14/06/2018, (IIT).
5. "The Virtual Human: In Silico Methods for Personalised Medicine", Prof. Peter Coveney, University College London; 8/07/2018, (IIT).
6. "Polymer drug delivery systems for lung delivery toward precision therapies in Cystic Fibrosis ", Dr Gabriella Costabile, Ludwig-Maximilians Universität Munich. 28/09/2018, (IIT)
7. "Structure-based anti-infective discovery" Prof. Anna K. H. Hirsch - Department of Drug Design and Optimization, Helmholtz Institute for Pharmaceutical Research (HIPS), Saarland University, Saarbrücken, Germany ,31/10/2018 (IIT):

8. "Precision Therapy Based on a Molecular Platform for RNA Therapeutics" Prof. Dan Peer, Tel Aviv University, 02/11/2018, (IIT)
9. "Doxil® - The first FDA Approved Nano-Drug Lessons Learned as Scientist, Developer and Entrepreneur", Prof. Yechezkel (Chezy) Barenholz, The Hebrew University Jerusalem, 02/11/2018, (IIT)
10. "Structure, Biophysics and Fragment-Based Lead Generation in Drug Discovery: AstraZeneca's Approach" Dr Maria M. Flocco, Global Head of Structural Biology, Biophysics & Fragment-Based Lead Generation, AstraZeneca, 19/11/2018 (IIT)
11. "Chemical proteome mining to fight multiresistant bacteria", Prof. Stephan Sieber, TU München 25/02/2019, HIPS
12. "Post-PKS Enzyme Complexes", Prof. Dr. Jürgen Rohr, University of Kentucky, 27/02/2019, HIPS seminar
13. "Carbohydrate-lectin interactions – What makes them unique?", Prof. Beat Ernst, University of Basel
14. "Antibiotics: Current situation and future perspectives"., Prof. Peter Hammann of Sanofi, Evotec and Gießen University From 02/03/2019 HIPS seminar: May 27th to May 29<sup>th</sup> 2019, HIPS seminar
15. "Structural Variation in Single Cells", Prof. Dr. Tobias Marschall, Max-Planck- Institut für Informatik 02/04/2019, HIPS seminar
16. "Epigenetic drug and assay development: inhibitors of Polycomb methyl readers, and novel methyltargeting reagents". Prof. Dr. Fraser Hof, University of Victoria, 06/06/2019, HIPS seminar.



**Università degli Studi di Genova**  
**Doctorate in**  
**Sciences and Technologies of**  
**Chemistry and Materials**



**Curriculum: Pharmaceutical, Food and Cosmetic Sciences**

**MARYAM HOOSHYARI**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*

**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*

**Advisor:** Prof.ssa Monica Casale

**Thesis Title:** Chemometrics Methods Applied to Non-Selective Signals in Order to Address Mainly Food, Industrial and Environmental

**Thesis abstract**

Chemometrics is a chemical discipline that uses mathematical and statistical methods in order to extract useful information from multivariate chemical data. Moreover, chemometrics is applied to correlate quality parameters or physical properties to analytical instrumental data such as calculating pH from a measurement of hydrogen ion activity or a Fourier transform interpolation of a spectrum. Aim of this thesis project is to develop new chemometric strategies for the elaboration and the interpretation of non-selective complex data in order to solve real problems in food, industry and environment fields.

## **ACTIVITY REPORT**

### **Research Activity**

***Research Period Abroad***

- 4-19 03/2017: Training on Fluorescence Spectroscopy at Department of Chemistry, Analytical Chemistry, Faculty of Science of Burgos University, Spain, under the supervision of Prof. M<sup>a</sup> Cruz Ortiz Fernandez.
- 22/06/2018 – 14/08/2018: PhD student Visitor at NIVA Institute, Oslo, Norway, under the supervision of Dr. Saer Samanipour.

## **Scientific Publications**

1. "Combining spectroscopic techniques and chemometrics for the interpretation of lichen biomonitoring of air pollution", *Chemosphere*, (2018), 198, 417-424. DOI: <https://doi.org/10.1016/j.chemosphere.2018.01.136>
2. "Combining excitation-emission matrix fluorescence spectroscopy, parallel factor analysis, cyclodextrin-modified micellar electrokinetic chromatography and partial least squares class-modelling for green tea characterization", *Journal of Pharmaceutical and Biomedical Analysis*, (2018), 159, 311-317. DOI: <https://doi.org/10.1016/j.jpba.2018.07.001>.
3. "The Effect of Extraction Methodology on the Recovery and Distribution of Naphthenic Acids of oilfield Produced Water", *Science of The Total Environment*, (2019), 652, 1416-1423. DOI: <https://doi.org/10.1016/j.scitotenv.2018.10.264>
4. "D-Optimal Design and PARAFAC as Useful Tools for the Optimisation of Signals from Fluorescence Spectroscopy Prior to the Characterisation of Green Tea Samples", *Food Analytical Methods* (2019), 12, 761-772. DOI: <https://doi.org/10.1007/s12161-018-01408-0>

## **Communications at Conferences**

### **Oral and Poster Communications:**

1. "Comparison between NIR spectroscopy and other analytical methods for the bio-monitoring of air pollution by lichens", M. Casale, P. Giordani, P. Malaspina, **M. Hooshyari**, M. Di Carro, ICNIRS 2017, The International Conference on Near Infrared Spectroscopy, 11th to 15th of June 2017, Copenhagen, Denmark; POSTER.
2. "D-Optimal Design to Optimize Fluorescent Signals from Solid and Liquid Samples of Green Tea and Their Subsequent Typification", **M. Hooshyari**, L. Rubio, M. Casale, S. Furnaletto, F. Turrini, L.A. Sarabia, M.C. Ortiz, 27th to 30th of June 2017, 9th Colloquium Chimiometricum Mediterranean; Arles, France; ORAL.
3. "Fluorescence Spectroscopy and Chemometric Techniques for Geographical Discrimination of Green Tea Samples", M. Casale, B. Pasquini, **M. Hooshyari**, S. Orlandini, M.C. Ortiz, L.A. Sarabia, S. Furlanetto, 10th to 14th of September 2017, XXVI National Conference of the Chemical Italian Society (SCI); Paestum (SA), Italy; POSTER.
4. "Effect of storage in plastic bottles on the quality of extra virgin olive oil", **Maryam Hooshyari\***, Eleonora Mustorgi, Cristina Malegori, Paolo Oliveri, Monica Casale. the ninth Giornate Italo-Francesi di Chimica scientific conference, 16th - 18th April 2018, Genova, Italy; POSTER.
5. "NIR spectroscopy, an efficient tool for evaluating and enhancing the quality of extra virgin olive oil", Monica Casale\*, **Maryam Hooshyari**, Eleonora Mustorgi, Cristina Malegori, Paolo Oliveri, VIII Italian Symposium of Spectroscopy NIR, 30th - 31st May 2018, Genova, Italy; POSTER.
6. "Near-Infrared Spectroscopy and Spectrofluorimetry combined with Chemometrics In Order to Determine the Performance Level of Gasoline Engine Oils", **M. Hooshyari\***, M. Casale, P. Oliveri, R. Leardi, 3rd International Conference and Exhibition on Petroleum, Refining and Environmental Technologies, PEFTEC; Rotterdam, Netherland, 22-23.05,2019; POSTER.
7. "PLS Regression Models for the Determination of EVOO Quality Parameters by NIR Spectroscopy: a Comparative Study", E. Mustorgi, M. Casale, **M. Hooshyari**, C. Malegori, P. Oliveri, M. Oteri, L. Mondello, 10th Colloquium Chimiometricum Mediterranean, Minorca, Spain 12-14.06.2019; POSTER.

8. "Spectroscopic Techniques Coupled with Chemometrics for the identification of Base Oil Type into Engine Oils, M. Casale, **M. Hooshyari**, C. Malegori, E. Mustorgi, P. Oliveri, R. Leardi, 10th Colloquium Chemiometricum Mediterranean, Minorca, Spain 12-14.06.2019; POSTER.
9. "Comparing Near Infrared Spectroscopy and Spectrofluorimetry in the Determination of Base Oil in Engine Lubricants", M. Casale, **M. Hooshyari**, C. Malegori, E. Mustorgi, P. Oliveri, R. Leardi, 19th International Council for NIR Spectroscopy Meeting, NIR2019, Gold Coast, Australia, 15-20.09.2019; POSTER.
10. "Application of PARAFAC on excitation–emission matrix fluorescence spectra for green tea characterization", E. Mustorgi, M. Casale, **M. Hooshyari**, P. Oliveri, C. Malegori, R. Bro, S. Furlanetto XXVIII Congress of the Analytical Chemistry Division Bari 22–26.09.2019; POSTER.
11. "Evaluation of analytical performances of quartz cuvettes and disposable glass vials for the determination of fame and tags in extra virgin olive oil", E. Mustorgi, M. Casale, C. Malegori, P. Oliveri, **M. Hooshyari**, L. Mondello, M. Oteri, XXVIII Congress of the Analytical Chemistry Division Bari 22 – 26.09.2019; POSTER.
12. "Characterization of base oils for engine lubricants by nir and fluorescence spectroscopies coupled with chemometrics", M. Casale, **M. Hooshyari**, C. Malegori, E. Mustorgi, P. Oliveri, XXVIII Congress of the Analytical Chemistry Division Bari 22 – 26.09.2019; ORAL.

## ***Courseware***

### ***Courses attended and passed***

#### ***Courses Given by Teachers of the UNIGE and IIT:***

1. Multivariate Analysis of Chemical Data, 3 Credits.
2. Introduction to The RAMAN Spectroscopy Applied to Materials, 2 Credits.
3. Mathematical Methods for Chemistry, 2 Credits.
4. Hit to Lead and Lead Optimization–Medicinal Chemistry, 1 Credit.

#### ***Courses Given by Invited Experts:***

1. Italian Language Course
2. Principles of Computer-aided Drug Design, Prof. Tiziano Tuccinardi from Centre for Biotechnology, Temple University, Philadelphia, One Credit.
3. Synthesis methods in solid state chemistry, Prof. Hans Flandorfer from University of Vienna, Dep. of Inorganic Chemistry – functional Materials, One Credit.
4. Environmental Accounting, Prof. Sergio Ulgiati from Parthenope University of Napoli, Department of Sciences and Technologies, One Credit.

### ***National and International Schools or Workshops***

1. 10th to 14th of April 2017 in Milan, Italy; 2nd edition of the Winter School of SISNIR in cooperation with the Council for Agricultural Research and Economics, CREA "The spectroscopic techniques: innovative tools to meet the new challenges for the future"

*Concepts of this school were included:*

- a. "A glance over a lifelong love affair" by Dr. Roberto Giangiacomo, SISNIR emeritus member, Milan ICNIRS Award 2009
- b. "The spectroscopic techniques: how, where, when and Council Management Committee, SISNIR Management Committee, UNIPD, Padua
- c. "RAMAN spectroscopy: basic principles" by Dr. Camilla Baratto, Senior Scientist, CNR-INO Brescia
- d. "IR spectroscopy: basic principles" by Prof. Elena Tamburini, UNIFE, SISNIR member, Ferrara
- e. "NIR spectroscopy: basic principles" by Prof. Elena Tamburini, UNIFE, SISNIR member, Ferrara
- f. "NIR on the GO" Prof. Paolo Berzaghi, ICNIRS Council Management Committee, SISNIR Management Committee, UNIPD, Padua
- g. "Chemometrics: basic principles of multivariate statistical analysis" by Prof. Michele Forina, SISNIR emeritus member, Genoa
- h. "Data processing: pre-treatments, approaches, software, applications" by Prof. Monica Casale, UNIGE – DiFar, SISNIR President, Genoa
- i. Lab trials on chemometrics by Dr. Stefania Barzaghi, CREA-FLC, SISNIR secretariat, Lodi
- j. "Two-dimensional correlation spectroscopy" by Dr. Stefania Barzaghi, CREA-FLC, SISNIR secretariat, Lodi
- k. "Multispectral and Hyperspectral Chemical Imaging Principles and Chemometrics" by Prof. Giorgia Foca, UNIMORE, SISNIR member, Reggio Emilia
- l. "Wood and restoration: updating innovative spectroscopic applications" by Dr. Anna Sandak, IVALSA-CNR, SISNIR member, S. Michele all'Adige
- m. "The time-resolved reflectance spectroscopy (TRS): basic principles, data processing and applications" by Prof. Alessandro Torricelli, PoLiMi, Milan, Dr. Lorenzo Spinelli, CNR, Milan Dr. Maristella Vanoli, CREA-IAA, Milan
- n. "The electron paramagnetic resonance spectroscopy( EPR): principles and applications" by Dr. Roberto Lo Scalzo, CREA-IAA, Milan
- o. "Imaging techniques combined with Hyperspectral Imaging – application trials" by Dr. Paolo Menesatti – Senior Scientist, CREA, Agricultural Engineering, Roma
- p. "The properties of water" by Dr. Roberto Giangiacomo, SISNIR emeritus member, Milan
- q. "Aquaphotomics: Past, Present and Future" by Dr. Tiziana M.P. Cattaneo, CREA-IAA, SISNIR member, Milan on behalf of Roumiana Tsenkova, Kobe University, Japan
- r. "Aquaphotomics in food science and agriculture" by Dr. Tiziana M.P. Cattaneo, CREA-IAA, SISNIR member, Milan.

2 "24<sup>th</sup> of May 2017 in Milan, Italy; Event: "NIR and PAT: a smart combination"

It was one day workshop focused on NIR spectroscopy for process monitoring which hold on by SISNIR (Società Italiana di Spettroscopia NIR) in collaboration with Università degli Studi di Milano and with patronage of ISPE ITALY Affiliate. Presentations were performed in subjects of:

- a. Real time chemical and physical analysis of tablet with spatially resolved spectroscopy and multipoint NIR push broom imaging technology" by Fabien Chauchard - Indatech
- b. "NIR Analysis in Natural Polymer Functionalization" by Gianmarco Polotti - Lamberti
- c. "Pharmaceutical Continuous Manufacturing Process: PAT applications for process monitoring." By Remo Simonetti
- d. "Monitoring of batch production of expanded polystyrene" by Erik Mantovani-Eni-Versalis



- e. "Building the product quality "by design" – Applications in the pharmaceutical and food industries." by Pierantonio Facco - UNIPD
  - f. "Application of NIR spectroscopy for monitoring granulation and blending in solid dosage form" by Emiliano Genorini - Viavi Solutions
  - g. "Hyperspectral Imaging for the On-line Characterization of E-waste: Towards Smart Demanufacturing Systems." By Nicoletta Picone - Italian National Research Council
  - h. NIR application to monitor an industrial process manufacturing additives for lubricant oils." Maria Concepción Cerrato Oliveros – Infineum
  - i. "Process monitoring in the baking industry: fusing NIR and process parameters to assure product quality" by Mario Li Vigni - CHEM-STAMP
  - j. Chemometrics in QbD and PAT contexts" by Marina Cocchi - UNIMORE
3. School of Experimental Design, 25-29 September 2017, Genoa.
  4. School of Chemometrics, 30 January-2 February 2017, Genoa (in Italian Language).
  5. School of Chemometrics, 29 May-1 June 2017, Genoa (in Italian Language).
  6. 07/05/2018 - 08/06/2018: "Copenhagen School of Chemometrics. CSC-2018", Copenhagen, Denmark:
    - a. Linear Models, Prof. Age Smilde and Dr. Federico Marini
    - b. Linear Algebra, Dr. Morten A. Rasmussen
    - c. Explorative Data Analysis, Prof. Rasmus Bro
    - d. Multivariate Regression, Dr. José Manuel Amigo.
    - e. Linear Classification, Dr. Davide Ballabio.
    - f. Variable Selection, Dr. Åsmund Rinnan.
    - g. Multivariate Curve Resolution by Dr. Anna de Juan.
    - h. Hyperspectral Image Analysis, Dr. José Manuel Amigo.

### **Other Activities**

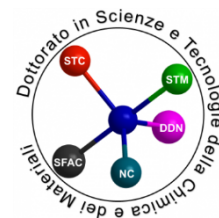
1. Seminars 1-4) Seminars of the SFAC PhD students attending the XXXI cycle; October 15<sup>th</sup> 2018, DIFAR, Viale Benedetto XV 3:
  - a. "Chemistry in the kitchen from traditional to molecular cooking". Dr. Giacchello Ilaria, PhD student at DIFAR-Università degli studi di Genova.
  - b. "Oral diseases and their treatment: an overview". Dr. Neduri Kartik, PhD student at DIFAR-Università degli studi di Genova.
  - c. "Five isoforms of N,N,N-tris(tert-butoxycarbonyl)-L-arginine depending on procedure and the investigation of their reactivity in esterification reactions". Dr. Taptue Gaby Brice, PhD student at DIFAR-Università degli studi di Genova.
  - d. "Deubiquitinase inhibition as therapeutic strategy". Dr. Zoppi Vittori, PhD student at DIFAR-Università degli Studi di Genova.
5. "Advances on first order algorithms for constrained optimization problems in Machine Learning"; Francesco Rinald from Università di Padova (Padova - Italia); October 19<sup>th</sup> 2018; Università di Genova, Via Dodecaneso 35 -.

6. "New perspectives for low temperature refrigeration with advanced magneto-caloric materials"; Prof. Julian G. Sereni, Low Temperature Division - Centro Atomico Bariloche - San Carlos de Bariloche - Argentina; 13 Novembre 2018 DCCI (Via Dodecaneso, 31, 16146 Genova GE).
7. "Anomalous transport properties in Weyl semimetals"; Federico Caglieris from Leibniz Institute for Solid State and Materials Research (IFW), Dresden, Germany; November 19<sup>th</sup> 2018, DIFI, Genova.
8. "Lipocalin-2 overexpression effects on bone and energy metabolism"; Sara Tavella from DIMES; January 16<sup>th</sup> 2018, Anatomia Umana.
9. "Il controverso ruolo della beta amiloide nella malattia di Alzheimer"; Roberta Ricciarelli from DIMES; Wednesday, January 30<sup>th</sup>, Anatomia Umana Via de Toni 14.
10. "Searching for superconductivity in graphite intercalated with hydrogen-based compounds"; Sébastien Cahen from Institut Jean Lamour, UMR 7198 CNRS - Université de Lorraine, Nancy, France; Feb 4<sup>th</sup> 2019 Dipartimento di Fisica.
11. "How to get much more information out of your date?"; Prof. Rasmus Bro from University of Copenhagen; Friday Feb 8<sup>th</sup> 2019, Department of Pharmacy.
12. "Definition of a new biological clock based on changes in energy metabolism"; Silvia Ravera from DIMES; February 13<sup>th</sup> 2019, Anatomia Umana Via de Toni 14.
13. "Introduction to Light-emitting diodes and Lasers based on Colloidal Semiconductor Nanocrystals"; Dr. Francesco Di Stasio Affiliation: ICFO (former), currently visiting scientist at the University of Genoa; February 14<sup>th</sup> 2019, DCCI Department of Chemistry and Industrial Chemistry University of Genoa
14. "Ormoni, interferenti endocrini ed omeostasi lipidica epatica"; Elena Grasselli from DISTAV; Wndsday, February 27<sup>th</sup> 2019, Anatomia Umana Via de Toni 14.
15. "Ask More from Chemistry - Analytical studies applied to Material Performances: an Industrial approach"; Marco Apostolo and Stefano Radice from Solvay Specialty Polymers; March 8<sup>th</sup> 2019, DCCI.
16. "The challenge of preserving metallic artefacts: obstacles and solution "; Emma Angelini from the Department of Applied Science and Technology of the Polytechnic of Turin; June 12<sup>th</sup> 2019 Department of Chemistry and Industrial.
17. "Caloric Effects in Magnetic Materials"; Prof. Hari Srikanth, 2019 IEEE Magnetics Distinguished Lecturer from University of South Florida (USA), Tuesday, September 10<sup>th</sup>, 2019, Aula 2 of the Department of Chemistry and Industrial.
18. Seminars 18-22 by the SFAC PhD students attending the XXXII cycle; October 15<sup>th</sup> 2019, DIFAR, Viale Benedetto XV 3:
  - a. "Astrochemistry: the chemistry of stars". Dr. Valeria Francesconi, PhD student at DIFAR-Università degli studi di Genova.
  - b. "Preliminary in vitro assays to evaluate anticancer drugs". Dr. Chiara Greco, PhD student at DIFAR-Università degli studi di Genova.
  - c. "Combination of conventional antibiotics with natural products: a promising strategy in overcoming antibiotic resistance". Dr. Francesca Pedrelli, PhD student at DIFAR-Università degli studi di Genova.

- d. "Production of biopharmaceutical proteins: particular case of the plants". Dr. Romeo Arago Dougue, PhD student at DIFAR-Università degli studi di Genova.



**Università degli Studi di Genova**  
**Doctorate in**  
**Sciences and Technologies of**  
**Chemistry and Materials**



**Curriculum: Nanochemistry**

**PALVASHA IJAZ**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2015*  
**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*  
**Advisors:** Liberato Manna (IIT), Roman Krahne (IIT), Iwan Moreels (IIT, University of Ghent), Maurizio Canepa (Unige)

**Thesis Title:** Ultrafast laser spectroscopy of novel fluorescent nanocrystals

**Thesis abstract**

Optical properties of colloidal semiconductor nanocrystals (NCs) have been widely investigated using optical spectroscopy techniques since their birth. In particular, low-temperature spectroscopy minimizes the additional complexity induced by thermal effects, and therefore has been extensively used to investigate the temperature dependent excitonic behavior of various semiconductor materials. It has been well established that the composition, structure and the nature of the NCs surface strongly influence their optical properties. Present PhD dissertation focuses on two main generations of semiconductor colloidal NCs, i.e. 2D metal chalcogenide nanoplatelets and lead halide perovskite NCs. The former generation of material demonstrate remarkable optoelectronic properties, with a narrow and homogeneously broadened emission linewidth (at room temperature), fast exciton recombination and high fluorescence quantum efficiency. These advantageous properties can be further tuned in heterostructures by growing another semiconductor on top or bottom facets (core/shell nanoplatelets), or on the lateral facets of the nanoplatelet (core/crown nanoplatelets) for instance CdSe/CdS/CdTe nanoplatelets. Due to the staggered band offset between CdSe and CdTe, we observed emission from an indirect transition around 650 nm. As CdS forms a barrier for hole relaxation between crown and core regions, the CdSe/CdS/CdTe yielded an additional emission peak from the CdSe core, in contrast with CdSe/CdTe core/crown nanoplatelets without a barrier. The resulting dual emission was investigated as a function of temperature. The different nature of both emission peaks (direct in CdSe vs. indirect across the CdSe/CdTe interface) yielded a spectrally and temporally stable indirect transition as a function of temperature, while the emission rate of the CdSe emission increased at lower temperatures, and the spectral position shifted to shorter wavelengths. The second generation of material studied here i.e. "lead halide perovskite" NCs is one of the most investigated semiconductor material in the last years due to their ease of preparation, broadly tunable band gap, near unity fluorescence quantum efficiency and excellent color purity. We carried out a comprehensive study of size, composition and surface

functionalization dependent optical properties of lead halide perovskite NCs. Contrary to most of the previous findings, we observe a single, narrow emission peak at low temperature for NCs with various sizes, compositions and surface coatings. Temperature-dependent photoluminescence (PL) and PL-lifetime data for different compositions (APbBr<sub>3</sub>, A=Cs, MA, FA) reveal that MA-based NCs were the most sensitive to temperature variations with least preservation of PL, featuring the highest thermal broadening of PL and longest lifetimes, whereas FA based NCs were the most resilient. Furthermore, a comparison of the photophysical properties of NCs having different surface coatings shows that their optical properties are strongly influenced by surface chemistry, with quaternary bromide capped NCs being the most stable samples at elevated temperature, as they retained the highest PL intensity. Considering all these results together, we provide unequivocal evidence that lead halide perovskite NCs exhibit no inhomogeneity in their PL and additionally their optical properties are strongly surface functionalization dependent.

## ACTIVITY REPORT

### *Research Activity*

#### *Research Period Abroad*

The research activity was mainly carried out at IIT

#### *Scientific Publications*

1. **Ijaz. P.** et al. Composition and Surface Functionalization dependent Optical Properties of Lead Halide Perovskite Nanocrystals (In preparation)
2. **Ijaz. P.** et al. Ultrafast laser spectroscopy of CdSe/CdS/CdTe core/crown nanoplatelets (in preparation).
3. Imran M, **Ijaz P**, Goldoni L, Maggioni D, Petralanda U, Prato M, Almeida G, Infante I, Manna L. Simultaneous Cationic and Anionic Ligand Exchange For Colloidally Stable CsPbBr<sub>3</sub> Nanocrystals. ACS Energy Letters. 2019, 4;4(4):819-24.
4. Imran M, **Ijaz P**, Baranov D, Goldoni L, Petralanda U, Akkerman Q, Abdelhady AL, Prato M, Bianchini P, Infante I, Manna L. Shape-Pure, Nearly Monodispersed CsPbBr<sub>3</sub> Nanocubes Prepared Using Secondary Aliphatic Amines. Nano letters. 2018, 1;18(12):7822-31.
5. Shamsi J, Dang Z, **Ijaz P**, Abdelhady AL, Bertoni G, Moreels I, Manna L. Colloidal CsX (X= Cl, Br, I) nanocrystals and their transformation to CsPbX<sub>3</sub> nanocrystals by cation exchange. Chemistry of Materials. 2017, 19;30(1):79-83.

### *Courseware*

#### *Courses attended and passed*

#### *B-type Courses Given by Teachers of the IIT*

1. Electronic properties of solids (3 credits) from 02/03/2016 to 16/05/2016 activated by Unige, *Speaker: Liberato Manna*

2. Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations (1 credit), *Speaker: Luca de Trizio*
  - Nanomaterials: Synthesis - methods and techniques
  - Nanomaterials: Synthesis - methods and techniques II
  - Post-synthesis Transformations: Cation Exchange Reactions
  
3. Basics of Crystallography and Diffraction by crystals (1 credit), *Speaker: Mirko Prato*
  - Symmetry, lattices, crystallographic systems and space groups
  - Crystallographic computing and the reciprocal lattice
  - Diffraction by crystals: theory and examples
  
4. Introductory course on transmission electron microscopy (1 credit), *Speakers: Rosaria Brescia, Zhiya Dang, Joka Buha, Roberto Marotta*
  - Introduction to transmission electron microscopy
  - Analytical electron microscopy
  - High-resolution TEM and in-situ TEM
  - Introduction to electron microscopy in biology, cryo (CryoEM) electron microscopy and electron Tomography
  
5. Nanoparticles characterization by Dynamic Light Scattering and Atomic Force Microscopy (3 credits) started from 13/01/2016 activated by Unige, *Speaker: Ranieri Rolandi*
  
6. Opto-Electronic Properties of Semiconductor Quantum Dots (1 credit), *Speaker: Iwan Moreels*
  - Electrons in Free Space and Bulk Crystals
  - Band Structure of Bulk Metals, Insulators and Semiconductors
  - Confinement in 1, 2 and 3 Dimensions
  - Optical Properties of Semiconductor Quantum Dots 06/07/2017
  
7. Laser-matter interactions: from fundamentals to applications" (3 credits) from 04/07/2017 to 25/07/2017 activated by Manuela Salvatori (IIT), *Speaker: Dr. Marti Duocastella*
  
8. Spectroscopies for chemical analysis (1 credit) from 26/09/17 to 28/09/17  
*Speaker: Francisco Palazon, Roman Krahné, Iwan Moreels*
  - Introduction to X-ray Photoelectron Spectroscopy
  - Introduction to NMR
  - Introduction to Raman

**A-type courses Given by invited experts (4 credits):**

1. "Magnetic hyperthermia: from fundamentals to biomedical applications", *Speaker: Dr. Francisco Terán*
  - iMdea Nanociencia, Ciudad Universitaria de Cantoblanco, 28049 Madrid, Spain

- Nanobiotecnología, CNB-CSIC-iMdea Nanociencia, Campus Universitario de Cantoblanco, Madrid, Spain ,05/05/2016 – 06/05/2016
- 2. “An introduction to nanoscale magnetism for biomedical applications”, Speaker: Neil Telling, Keele University, UK.
  - Magnetism at nanoscale.
  - Biomedical applications of magnetic nanoparticles, 23/05/2017 – 24/05/2017
- 3. “From Crystallography to Imaging”, Speaker: Cinzia Giannini, University of Bari 23/04/2018 – 24/04/2018
- 4. “Nanoparticle Chemistry for the use of energy Conversion and Theranostics”, Speaker: Prof. Clemens Burda, Case Western Reserve University 21/06/2018 – 22/06/2018

### ***National and International Schools or Workshops***

1. International WE-Heraeus-Physics School on “Exciting Nanostructures: Probing and Tuning the Electronic Properties of Confined Systems”, July 17-21, 2017 at the Physikzentrum Bad Honnef (Germany)

### ***Seminars Attended***

5. Materials for therapy: Cesium Oxide nanoparticles as novel antioxidant drugs. Prof. Enrico Traversa 04/02/2016
6. Ionic bonding and the effect of electron repulsion on the band structure, Liberato Manna, 08/06/2016
7. Van der Waals Assembly of 2D materials for device applications, Dr. Gwan-Hyoung Lee, 16/01/2017
8. Colloidal Double Quantum Dots, Dan Oron, 14/02/2017
9. Theatrocracy: the communication in the modern age. Stefano Amoroso, 02/03/2017
10. High-throughput design of doped colloidal nanocrystals Emory Chan 01/06/2017
11. Synthetic methodology for colloidal nanomaterials: limitations and opportunities, Dmitri Talapin, 26/05/2017
12. The Role of membrane curvature at the Nano-Bio interface, Prof. Bianxiao CUI, 12/09/2017
13. Standardization methods for the synthesis of single-core and multi-core magnetic nanoparticles for medical applications. Helena Gavilan Rubio 02/10/2017
14. Electron Microscopy Facility Seminar: “Aberration-corrected STEM: sub-Å resolution imaging, atomic-resolution elemental mapping, and vibrational spectroscopy”, Dr. Ondrej L. Krivanek, Nion R&D Company and Arizona State University, USA 04/10/2017
15. Graphene and other 2D related materials interface engineering for highly efficient and stable organic and perovskite solar cells Dr. Emmanuel Kymakis, Center of Materials Technology & Photonics and Electrical Engineering Department, Technological Educational Institute (TEI) of Heraklion, Crete, Greece 14/11/2017
16. Scattering-Type Scanning Near-Field Optical Microscopy for various applications, Dr. Philip Schaefer 27/02/2018
17. Photophysics and photonic applications of alternative plasmonic nanomaterial, Dr. Francesco Scotognella 05/04/2018
18. Nanoparticle Chemistry for the use of energy conversion of Theranostics Prof. Clemens Burda, 21/06/2018

19. Attosecond microscopy and control of matter down to the nucleus, Prof. Fabrizio Carbone  
19/10/2018
20. Workshop Public Speaking / Adding visuals to slide-based presentations Jacopo Pasotti Journalist  
– Science Communicator. March 26-27, 2018

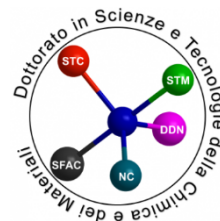
**Others**

- ✓ Training on Edinburg instrument for PL, TCSPC and QY measurements
- ✓ Training on Cryosat for low temperature measurements
- ✓ Analysis work on Igor Pro software





**Università degli Studi di Genova**  
**Doctorate in**  
**Sciences and Technologies of**  
**Chemistry and Materials**



**Curriculum: Chemical Sciences and Technologies**

**PAOLA LOVA**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*  
**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*  
**Advisor:** Prof. Davide Comoretto  
**Thesis Title:** Flory-Huggins Photonic Sensors

**Thesis abstract**

This thesis aims to the design, fabrication and characterization for new polymer based photonic crystal devices for application including sensing, and light management. Photonic crystals are composite materials made of media with different refractive index periodically arranged into a sub-micrometric lattice. The interaction between light and these lattices generates a photonic band structures, characterized by frequency region allowed and forbidden to photon propagation. The latter are called photonic band-gaps and are widely employed to create functional devices. Historically, photonic crystals were made by inorganic media which provide large dielectric contrast, but they are characterized by time-consuming and hardly scalable fabrication. This thesis work aims to the demonstration of proof-of-concept polymer and hybrid photonic crystals manufactured by easy to scale-up solution-based processes to overcome the limitation characteristic of inorganic structures.

**ACTIVITY REPORT**

***Research Activity***

***Research Period Abroad***

- Nanyang Technological University, Singapore, 09-22 January 2017 - Fabrication and Characterization of polymer photonic crystals embedding MA PbX<sub>3</sub> perovskite
- European Synchrotron Radiation Facility (ESRF), Grenoble, France, 21-26 February 2018 – Time resolved wide angle X-ray scattering of Vapor induced Poly(p-phenylene oxide) crystallization in selective photonic crystals sensors. EXP. N. MA-3272
- University of Groningen, Zernike institute for advanced materials, 20-26 January 2018 - Steady state wide angle X-ray scattering of Vapor induced Poly(p-phenylene oxide) crystallization in selective photonic crystals sensors.
- Nanyang Technological University, Singapore, 23 April 2018 - 06 May 2018 - Fabrication and Characterization of polymer photonic crystals embedding MA PbX<sub>3</sub> perovskite

- European Synchrotron Radiation Facility (ESRF), Grenoble, France, 11-14 November 2016 – Time resolved wide angle X-ray scattering of Vapor induced Poly(p-phenylene oxide) crystallization in selective photonic crystals sensors. EXP. N. MA-3272
- University of Groningen, Zernike institute for advanced materials, 20-26 January 2018 - Steady state wide angle X-ray scattering of Vapor induced Poly(p-phenylene oxide) crystallization in selective photonic crystals sensors.
- Strasbourg University, Supramolecular Science and Engineering Institute, 11/17 November 2018 – AFM and XPS investigations of amorphous and clathrate Poly(p-phenylene oxide) thin films.

### **Scientific Publications**

1. **Lova, P.;** Bastianini, C.; Giusto, P.; Patrini, M.; Rizzo, P.; Guerra, G.; Iodice, M.; Soci, C.; Comoretto, D. Label-free vapor selectivity in poly(p-phenylene oxide) photonic crystal sensors. *ACS Appl. Mater. Interfaces* 2016, 8, 31941–31950.
2. Manfredi, G.; **Lova, P.;** Di Stasio, F.; Krahne, R.; Comoretto, D. Directional fluorescence spectral narrowing in all-polymer microcavities doped with cdse/cds dot-in-rod nanocrystals. *ACS Photonics* 2017, 4, 1761–1769.
3. **Lova, P.;** Grande, V.; Manfredi, G.; Patrin, M.; Herbst, S.; Würthner, F.; Comoretto, D. All-polymer photonic microcavities doped with perylene bisimide j-aggregates. *Adv. Opt. Mater.* 2017, 5, 1700523.
4. Manfredi, G.; **Lova, P.;** Di Stasio, F.; Krahne, R.; Comoretto, D. In Directional fluorescence shaping and lasing in all-polymer microcavities doped with cdse/cds dot-in-rod nanocrystals, 2017 European Conference on Lasers and Electro-Optics and European Quantum Electronics Conference, Munich, 2017/06/25, 2017; Optical Society of America: Munich, p CK\_10\_12.
5. **Lova, P.;** Cortecchia, D.; S. Krishnamoorthy, H.N.; Giusto, P.; Bastianini, C.; Bruno, A.; Comoretto, D.; Soci, C. Engineering the emission of broadband 2d perovskites by polymer distributed bragg reflectors. *ACS Photonics* 2018, 5, 867-874.
6. Manfredi, G.; **Lova, P.;** Di Stasio, F.; Rastogi, P.; Krahne, R.; Comoretto, D. Lasing from dot-in-rod nanocrystals in planar polymer microcavities. *RSC Advances* 2018, 8, 13026-13033.
7. Giusto, P.; **Lova, P.;** Manfredi, G.; Gazzo, S.; Srinivasan, B.; Radice, S.V.; Comoretto, D. Colorimetric detection of perfluorinated compounds by all-polymer photonic transducers *ACS Omega* 2018, 3, 7517-7522.
8. **Lova, P.;** Manfredi, G.; Comoretto, D. Advances in functional solution processed planar one-dimensional photonic crystals. *Adv. Opt. Mater.* 2018, 6, 1800730-1800726.
9. **Lova, P.** Selective polymer distributed bragg reflector vapor sensors. *Polymers* 2018, 10, 1161.
10. **Lova, P.;** Robbiano, V.; Cacialli, F.; Comoretto, D.; Soci, C. Black gas by metal-assisted chemical etching. *ACS Appl Mater Interfaces* 2018, 10, 33434-33440.
11. **Lova, P.;** Comoretto, D. Label-free vapor selectivity by polymer-inorganic composite photonic crystals sensors. *AIP Conf. Proc.* 2018, 1981, 020097.
12. Martinelli, A.; Alberti, S.; Caratto, V.; **Lova, P.;** Locardi, F.; Pampararo, G.; Villa, S.; Ferretti, M. Structural studies on copper and nitrogen doped nanosized anatase. In *Zeitschrift für Kristallographie - Crystalline Materials*, 2018; Vol. 233, p 867.
13. **Lova, P.;** Manfredi, G.; Bastianini, C.; Mennucci, C.; Buatier de Mongeot, F.; Servida, A.; Comoretto, D. Flory-huggins photonic sensors for the optical assessment of molecular diffusion coefficients in polymers. *ACS Appl. Mater. Interfaces* 2019, 11, 16872-16880.
14. Iasilli, G.; Francischello, R.; Lova, P.; Silvano, S.; Surace, A.; Pesce, G.; Alloisio, M.; Patrini, M.; Shimizu, M.; Comoretto, D., et al. Luminescent solar concentrators: Boosted optical efficiency by polymer dielectric mirrors. *Mater. Chem. Front.* 2019, 3, 429-436.

15. **Lova, P.;** Giusto, P.; Stasio, F.D.; Manfredi, G.; Paternò, G.M.; Cortecchia, D.; Soci, C.; Comoretto, D. All-polymer methylammonium lead iodide perovskite microcavity. *Nanoscale* 2019, 11, 8978-8983
16. **Lova, P.;** H. Megahd, C.; Comoretto, D. Thin Polymer Films: Simple Optical Determination of Molecular Diffusion Coefficients (Submitted)
17. **Lova, P.;** Comoretto, D. Tailoring the Properties of Polymers for Photonic Applications with Optical Nanocomposites. *AIP Conf. Proc.* (In Press).
18. **Lova, P.;** H. Megahd, Comoretto, D. A New Method for the Determination of Molecular Diffusion Coefficient in Polymer Films by Simple UV-Vis Spectroscopy. *AIP Conf. Proc.* (In Press).

### ***Communications at Conferences***

#### ***Oral communications:***

1. FisMat 2019
  - **P. Lova,** P. Giusto, F. Di Stasio, G. Manfredi, G. M. Paternò, D. Cortecchia, C. Soci, D. Comoretto. Reshaping Hybrid Perovskites Emission with Flexible Polymer Microcavities
  - **P. Lova,** H. Megahd, D. Comoretto. All-polymer Planar Photonic Crystals as an Innovative Tool for the Analysis of Air
2. ICSAAM 2019
  - **P. Lova,** H. Meghad, D. Comoretto. A New Method for the Determination of Molecular Diffusion Coefficient in Polymer Films by Simple UV-Vis Spectroscopy
  - **P. Lova,** D. Comoretto. Tailoring Optical and Mechanical Properties of Polymers for Photonic applications with Optical Nanocomposites
3. Nordic Italian Polymer Future 2019
  - **P. Lova,** D. Comoretto. A Simple Optical Method for the Assessment of Molecular Diffusion Coefficients and Sensing Using Polymer Thin Films
4. EPF 2019
  - **P. Lova,** A. Servida, D. Comoretto. Determination of Diffusion Coefficients and Sensing in Polymer Films by UV-Vis Spectroscopy
5. EOSAM 2018
  - **P. Lova,** D. Cortecchia, H. N. S. Krishnamoorthy, P. Giusto, C. Bastianini, A. Bruno, D. Comoretto, C. Soci. Reshaping White Light Emission from 2D Perovskites with Flexible Photonic Crystals
  - **P. Lova,** D. Comoretto. All-polymer Distributed Bragg Reflectors as Innovative and Powerful Chromatic Sensors
6. NANOPHOTONICS 2018
  - **P. Lova,** A. Servida, D. Comoretto. Polymer Distributed Bragg Reflectors: an Old Structure with Unexpected Sensing Capabilities
7. Polymer Crystallization Workshop 2018
  - **P. Lova,** A. Servida, D. Cavallo, G. Portale, D. Comoretto. Polymer Photonic Crystal Sensors
8. TOP 2018
  - **P. Lova,** D. Comoretto. Label-Free Vapor Selectivity by Polymer-Inorganic Composite Photonic Crystals Sensors (Oral)
9. XXIII CONVEGNO NAZIONALE AIM 2018
  - **P. Lova,** D. Comoretto, Polymer Photonic Crystals Sensors
10. EUPOC 2018, European Polymer Conference 2018
  - **P. Lova,** M. Olivieri, D. Cavallo, M. Viviani, G. Portale, A. Servida, D. Comoretto. Simple UV-VIS Study of Polymer-Molecule Supramolecular Interactions: Assessment of Diffusion Coefficients and Crystallinity in Polymer Films

#### 11. MACROGIOVANI 2017

- **P. Lova**. Polymer Photonic Crystals Sensors
- G. Manfredi, P. Lova, P. Perkhun, A. Surace, D. Comoretto. Polymer and Hybrid Materials for Photonic Crystals

#### 12. EMRS FALL 2017

- **P. Lova**, V. Grande, G. Manfredi, M. Patrini, S. Herbst, F. Würthner, D. Comoretto. All-Polymer Microcavities Doped with Perylene Bisimide J-Aggregates
- **P. Lova**, G. Manfredi, A. Servida, D. Comoretto. Sensing and Assessment of Molecular Diffusion Parameters by Polymer Photonic Crystals.

#### 13. EPF 2017

- **P. Lova**, G. Manfredi, S. Silvano, P. Giusto, D. Comoretto. Polymers for Photonic Devices

#### 14. Fotonica 2017 – 19o Convegno Italiano delle Tecnologie Fotoniche 3-5 May 2017, Padova, Italy

- **P. Lova**, G. Manfredi, S. Silvano, P. Giusto, D. Comoretto. All-polymer Photonic Crystal Sensors

#### **Poster Communications:**

##### 1. XXIII CONVEGNO NAZIONALE AIM 2018

- **P. Lova**, G. Pesce, M. Olivieri, M. Alloisio, and D. Comoretto. Polymers for Photonics

##### 2. WORKSHOP on ITALIAN-NORDIC POLYMER FUTURE

- **P. Lova**, G. Manfredi, A. Servida, D. Comoretto. Polymer Multilayered Photonic Crystals Vapor Sensors
- G. Manfredi, A. Surace, S. Silvano, **P. Lova**, D. Comoretto. Polymer and Hybrid Photonic Crystal Structures

#### **Congresses Attended**

1. FisMat 2019, Italian national conference on the physics of matter 2019, 30 September - 4 October 2019, Catania, Italy
2. ICSAAM 2019, The 9th International Conference on Structural Analysis of Advanced Materials, 12-15 September 2019
3. Nordic Italian Polymer Future 2019, 3-4 September 2019, Copenhagen, Denmark.
4. EPF 2019, European Polymer Federation Congress 2019, 9-14 June, Crete, Greece
5. EOSAM 2018, European Optical Society Annual Meeting 2018, 8-12 October 2018, Delft, Netherland
6. NANOPHOTONICS 2018, , Rome, Italy
7. Polymer Crystallization Workshop, 1-3 September 2018, Genova, Italy
8. TOP 2018 - Times of Polymers (TOP) & Composites 2018, 17-21 June 2018, Ischia, Italy
9. XXIII CONVEGNO NAZIONALE AIM, 9-12 September 2018, Catania, Italy
10. EUPOC 2018, European Polymer Conference 2018, 20-24 May 2018, Como, Italy
11. MACROGIOVANI 2017, 22-23 June 2017, Trento, Italy
12. WORKSHOP on ITALIAN-NORDIC POLYMER FUTURE, 14–15 September 2017, Pisa, Italy
13. EMRS FALL 2017 - Fall Meeting- European Material Research Society Fall Meeting, 18-21 September 2017, Warsaw, Poland
14. EPF 2017 - EUROPEAN POLYMER FEDERATION CONGRESS 2017, 2-7 July 2017, Lyon, France
15. Fotonica 2017 – 19o Convegno Italiano delle Tecnologie Fotoniche 3-5 May 2017, Padova, Italy

## Courseware

### **Type B courses:**

1. Analisi multivariata dei dati chimici (3 CFU)
2. Electronic Structure of Solids (3 CFU)
3. Material Organici per la Fotonica (2 CFU)
4. Proprietà ottiche dei Materiali (3 CFU)

### **Type A courses:**

1. Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials & Novel Materials for energy storage and conversion, Prof. Dr. Thomas Fässler, 11 May 2017, DCCI
2. Probing Matter with Synchrotron Radiation, Dott. Luigi Paolasini, 28-29 May 2019, DCCI
3. Environmental Accounting, Prof. Sergio Ulgiati (Parthenope University of Napoli, Department of Sciences and Technologies), 6-7 Maggio 2019
4. Phase diagrams of liquid-liquid demixing and polymer crystallization, Wenbing Hu, 3-4 July 2019

### **Seminars**

1. Sviluppo di nuovi materiali per olografia: dalla Molecola al Materiale, Andrea Bianco, 03 March 2017, DIFI
2. Fotopolimeri in astronomia, Alessio Zanutta, 03 March 2017, DIFI
3. Dal problema astronomico alla strumentazione: essere a meta' tra scienza e tecnologia, Marco Landoni, 03 March 2017, DIFI
4. Synthesis of high permittivity nanoparticles by hydrothermal and solvothermal methods, Vincenzo Buscaglia, 29 March 2017, ICMATE Genova
5. Polymer-based composites: Process-Structure-Properties Relationship, Paola Stagnaro, 29 March 2017, ICMATE Genova
6. Finite elements method modelling of dielectric and ferroelectric properties of composite systems, Leontin Padurariu, 29 March 2017, ICMATE Genova
7. Electrical properties of chitosan-based composites: toward active dielectrics for flexible electronics, Lavinia Curecheriu, 29 March 2017, ICMATE Genova
8. All-polymer nanophotonics: from lasers to sensors, Davide Comoretto 29 March 2017, ICMATE Genova
9. Atomic Structure and mass production of size selected nanoparticles (clusters). Richard. E. Palmer, 30 May 2017, DIFI
10. Novel small molecules, targets, and strategies in anti-infective development, Prof. Jason K. Sello, 3 July 2017, DCCI.
11. Introduction to transmission electron microscopy, Rosaria Brescia, 10 April 2017, IIT Morego
12. Materiali Organici Nanostrutturati a base di Carbonio, Azoto e Boro, Paolo Giusto, 29 November 2018
13. HIBRYD MAGNETIC NANO-ARCHITECTURE FOR APPLICATION IN BIOMEDICINE AND ENERGY, Davide Peddis, 18 gennaio
14. Colloidal Semiconductor Nanocrystals for Optoelectronics, Francesco Di Stasio, 7 Febbraio 2019, DCCI
15. Introduction to Light-emitting diodes and Lasers based on Colloidal Semiconductor Nanocrystals, Francesco di Stasio, 14 February 2019
16. Ask More From Chemistry, Solvay, 8 Marzo 2019, DCCI

### ***Seminars given, Classes, Outreach and Divulgation***

1. 29/01/2018 - Divulgation lecture on “Il Colore strutturale” to Primo Levi Institute, Ronco Scrivia.
2. 05/03/2018 - Front Class at UNITE (Università della terza età) on “Il Colore Strutturale e i Cristalli fotonici”, Genova.
3. 08/04/2019 - Center for Nano Science and Technology (CNST), Italian Institute of Technology, Monday Talk on: “Polymer Photonic Crystals”
4. 03/07/2019 – Università di Napoli Federico II on “Polymer Photonic Crystals, from light management applications to smart tools for pollutant recognition and determination of molecular diffusion coefficients”

### ***National and International Schools or Workshops***

1. 8<sup>th</sup> EPF Summer School – Transport Phenomena in Polymers and Hybrid Materials, 14-19 May 2017, Gargnano, Italy
2. Optical Characterization of Photonic Structures, International School, 06-08 June 2017, Pisa, Italy
3. 11<sup>th</sup> International School on Hybrid and Organic Photovoltaics 03-05 September 2017, Arbatax, Italy
4. 4th School on Advanced Materials for Photonics, Electronics and Bioelectronics 05-07 September 2017, Arbatax, Italy
5. Macrogiovani 2017, 22-23 May 2017, Trento, Italy, Photonic Devices for Biocomponents, International Workshop, 5-6 June 2017, Pisa, Italy, Italian-Nordic Polymer Future, 14-15/09/2017, Pisa, Italy, Italian Institute of Technology (IIT), Center for Nano Science and Technology (CNST) Winter Workshop 2017, Bormio (SO) 18-20 December 2017.

### ***Other Activities***

#### *Referee activity for:*

- MDPI (Chemosensors, Materials, Ceramics, Crystals, Sensors, Diagnostic)
- Wiley VCH (Advanced Materials)
- American Chemical Society (ACS Applied Materials Interfaces)
- Journal of the electrochemical Society (ECS Journal of Science and Technology)
- Royal Society of Chemistry (RCS Advances)

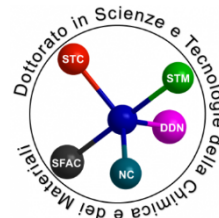
#### *Conference Organization*

- Macrogiovani 2020, June 2020, Genova, Italy. (Scientific and Organizing Committee)
- Macrogiovani 2019, July 2019, Napoli, Italy. (Scientific and Organizing Committee)  
<https://www.aim.it/macrogiovani2019>
- Macrogiovani 2018, 14-15 June 2018, Fisciano, Salerno, Italy. (Scientific and Organizing Committee)
- <https://cdn.website-editor.net/0ca4eb8b03aa46b6ae033a2d167e3bd8/files/uploaded/Macrogiovani%25202018.pdf>
- Polymer Crystallization Workshop, 1-3 September 2018, Genova, Italy. (Organizing Committee)



Università degli Studi di Genova

Doctorate in  
Sciences and Technologies of  
Chemistry and Materials



Curriculum: Scienze e Tecnologie Chimiche

EMANUELA MANFREDI

**Start of the Doctorate Program.** November 1<sup>st</sup>, 2016  
**End of the Doctorate Program:** October 31<sup>st</sup>, 2019  
**Advisors:** Prof. Giovanni Petrillo, Prof.ssa Silvana Dellepiane

**Thesis Title:** Elaborazioni digitali di tecniche fotografiche: applicazioni innovative ai materiali dell'arte come guida per interventi di restauro

## ACTIVITY REPORT

### *Research Activity*

The research activity was mainly carried out at the Department of Chemistry and Industrial Chemistry, University of Genova.

#### **Scientific Publications**

1. Moggia R., Brunetto A., Franceschi E., **Manfredi E.**, Manfrinetti P., Petrillo G., Dellepiane S., Sista A., *Combinazioni di laser e solvent-gel sulle formelle policrome ad olio su lamina metallica dei Misteri del Rosario di Chiusanico*, Conference Book of APLAR 6, applicazioni laser nel restauro, 14<sup>th</sup>-15<sup>th</sup> September 2017, Florence
2. **Manfredi E.**, Petrillo G., Dellepiane S., *Identification of artistic pigments: a comparison of different approaches to image acquisition and analytical data processing*, Book of Abstract of MERCK & ELSEVIER Young Chemists Symposium, November 19<sup>th</sup> – 21<sup>st</sup> 2018, Rimini
3. **Manfredi E.**, Petrillo G., Dellepiane S., *A novel digital-camera characterization method for pigment identification in Cultural Heritage*, Book of Abstract of CCIW 2019, IAPR The Seventh Computational Color Imaging Workshop, 27-29 March 2019, Chiba, Japan.

## ***Communications at Conferences***

### ***Oral communications:***

1. "APLAR 6, applicazioni laser nel restauro", September, 14-15, 2017, Florence.
2. "CCIW 2019, IAPR The Seventh Computational Color Imaging Workshop", March 27-29, 2019, Chiba, Japan.
3. XVIII Congresso Nazionale di Chimica dell'Ambiente e dei Beni Culturali, June, 24-27, 2019, Urbino.

### ***Poster Communications:***

1. "Scientia ad Artem, workshop", 8<sup>th</sup> June 2017, Florence
2. "XVII Congresso Nazionale di Chimica dell'Ambiente e dei Beni Culturali, June, 24-27, 2018, Genoa.
3. "MERCK & ELSEVIER Young Chemists Symposium", November, 19-21, 2018, Rimini

## ***Congresses Attended***

1. "APLAR 6, applicazioni laser nel restauro", September, 14-15, 2017, Florence
2. "X Congresso Nazionale AIAR, February, 14-17, 2018, Turin
3. "XVII Congrso Nazionale di Chimica dell'Ambiente e dei Beni Culturali, June, 24-27, 2018, Genoa.
4. "MERCK & ELSEVIER Young Chemists Symposium", November, 19-21, 2018, Rimini.
5. XVIII Congresso Nazionale di Chimica dell'Ambiente e dei Beni Culturali, June, 24-27, 2019, Urbino.

## ***National and International Schools or Workshops***

1. Scientia ad Artem", workshop, 8th June 2017, Florence
2. Il Scuola AIAR, Centro di Conservazione e Restauro "La Venaria Reale", 12th-13th February 2018, Turin
3. Scuola di Chemiometria, Analisi Multivariata, 21-25 January 2018, Genoa.
4. Scuola di Chemiometria, Disegno Sperimentale 27-31 May 2019, Genoa.

## ***Courseware***

### ***Courses attended and passed***

1. Analisi multivariata dei dati chimici (3 CFU)
2. Optical properties of materials (3 CFU)
3. Corrosione e Protezione dei Materiali (type F course 6 CFU)
4. Materiali funzionali e strutturali inorganici (type F course 6 CFU)
5. Scienze delle superfici (3 CFU)
6. Materiali Funzionali Strutturali Inorganica (type F course 6 CFU)
7. Electronic Structure of Solids (3 CFU)
8. Spectroscopies for chemical analysis (Module 5 of the Nanochemistry School, 1 CFU1)

### ***Courses Given by invited experts:***

1. Superfici ed interfacce in sistemi metallo-ceramici, Prof. Alberto Passerone, 16-19/03/2017)
2. Chemistry and Physics of Materials Science of Borides and particularly of Metal Boron Carbides, Prof. Peter Rogl, University of Vienna, June, 11 and 13, 2018



### ***Seminars Attended***

1. Mele P., On research activities at Muroran Institute of Technology, Genova, 24/07/ 2017.
2. Locardi F., Analisi termica accoppiata alla gas cromatografia e spettrometria di massa. Un potente strumento per le caratterizzazioni di materiali, Genova, 13/06/2017.
3. PHD students as a bridge between Science and society, Genova 27/10/2017.
4. Il progetto di restauro: cultura e metodo, 7th November, 2018, Genoa.
5. Laboratory of pigment and dye, March-April 2018," Dipartimento di Chimica e Chimica Industriale", Genoa
6. Apostolo M., Radice S., Ask More from Chemistry-Analytical studies applied to Material Performances: an industrial approach, 8th March 2019, Genoa.
7. Lotti N., Design of new biopolyesters for biomedicine and sustainable food-packaging, 02/04/ 2019, Genoa.
8. Angelini E., The challenge of preserving metallic artefact: obstacles and solution, 12/06/2019, Genoa.
9. Tassano E., Biocatalysis in medicinal chemistry, 4th October 4, 2019, Genoa.

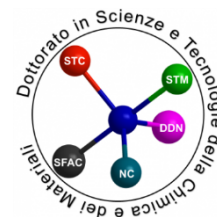
### ***Other Activities***

Lectures and courses given:

- Lessons about color at the Dipartimento di Chimica e Chimica Industriale, Genoa, 24th May 2017 and 13th May 2019
- course "Elaborazione digitale d'immagini storico-artistiche", delivered by Professor Silvana Dellepiane, in Department of Naval, Power, Electronics and Telecommunications Engineering, Università degli Studi di Genova, in date: 4th and 18th May 2017, 24th May 2018 and 16th May 2019.
- Lesson about colorimetry "Introduzione alla colorimetria dei beni culturali", Summer School 2019, Tecniche diagnostiche applicate ai beni culturali, 4th June 2019, Department of Chemistry and Industrial Chemistry, Università di Genova



Università degli Studi di Genova  
Doctorate in  
Sciences and Technologies of  
Chemistry and Materials



Curriculum: Chemical Sciences and Technologies

**ANGELA PAGANO**

**Start of the Doctorate Program:** November 1<sup>st</sup>, 2016  
**End of the Doctorate Program:** October 31<sup>st</sup>, 2019  
**Advisor:** Prof. Giovanni Petrillo

**Thesis Title:** Nitroheteroaromatics via Annulation with Nitro-1,3-butadienes: Synthesis and Applications

**ACTIVITY REPORT**

***Research Activity***

Erasmus+ Mobility for Traineeship at the Department of Chemistry of University of York (U.K.) under the supervision of Dr. William Unsworth, October 15th 2018– April 12th 2019

Traineeship title: “New catalytic methods for the preparation of heterocycles and spirocycles”

***Scientific publications***

Original publications on ISI Journals:

1. Ho, H. E.; **Pagano, A.**; Rossi-Ashton, J. A.; Donald, J. R.; O’Brien, P.; Taylor, R. J. K.; Unsworth, W. P. “Visible-Light-induced Intramolecular Charge Transfer in the Radical Spirocyclisation of Indole-tethered Yrones” *Chemical Science*, 2019, submitted.
2. Benzi, A.; Bianchi, L.; Maccagno, M.; **Pagano, A.**; Petrillo, G.; Tavani, C. “Sequential annulations to interesting novel pyrrolo[3,2-c]carbazoles” *Molecules*, 2019, 24, 3802; doi:10.3390/molecules24203802
3. **Pagano, A.**; Mancinelli, M.; Bianchi, L.; Giorgi, G.; Maccagno, M.; Petrillo, G.; Tavani, C. “Nitrobutadienes as powerful benzannulating agents: an unprecedented easy access to rare nitroindoles” *Tetrahedron*, 2019, 75, 4506.
4. **Pagano A.**, Marotta E., Mazzanti A., Petrillo G., Tavani C. and Mancinelli M. “Stereodynamic Analysis of New Atropisomeric 4,7-Di(naphthalen-1-yl)-5, 6-dinitro-1H-indoles” *Synlett*, 2018, 29, 2161.

## **Communications at Conferences**

### **Oral communications:**

1. **Pagano, A.**; Mancinelli, M.; Bianchi, L.; Maccagno, M.; Petrillo, G.; Tavani, C. "Conjugate Dinitrobutadienes As Valuable C4 Building-Blocks For The [4+2] Benzannulation Of Pyrrole" – ISOS, 2019, Gargnano (BS), Italy
2. Bianchi L., Giorgi G., Maccagno M., **Pagano A.**, Petrillo G., Tavani C. "Nitrobutadienes: suitable substrates for the original synthesis of novel polyfunctional indole derivatives" - IX Giornate Italo-Francesi di Chimica, April 16th-18th, 2018, Genova (Italy).
3. Bianchi L., Giorgi G., Maccagno M., **Pagano A.**, Petrillo G., Tavani C. "From dinitrobutadiene building-blocks to nitroindoles: an appealing access to otherwise not easily attainable functionalized heterocycles" – XVII Merck Young Chemists Symposium, November 13th-15th, 2017, Milano Marittima (Italy).
4. Bianchi L., Giorgi G., Maccagno M., **Pagano A.**, Petrillo G., Tavani C. "An appealing access to otherwise not easily attainable nitro-functionalized indoles" – La Giornata della Chimica Ligure, October 20th 2017, Genova (Italia)

### **Poster communications**

1. **Pagano A.**, Ho H. E., Taylor R. J. K., Unsworth W. P. "Visible-Light-induced Intramolecular Charge Transfer in the Radical Spirocyclization of Indole-tethered Ynones", 10th Eurasian Meeting on Heterocyclic Chemistry, September 15th-19th 2019, Milano Marittima (Italy).
2. **Pagano A.**, Ho H. E., Taylor R. J. K., Unsworth W. P. "Visible-Light Promoted Dearomatizing Spirocyclizations of Ynone-Tethered Indoles", XXXIX Convegno Nazionale della Divisione di Chimica Organica della Società Chimica Italiana, September 8th-12th 2019, Torino (Italy).
3. **Pagano A.**, Petrillo G. "Unprecedented nitroindoles as the result of an original benzannulation onto pyrrole with nitrobutadienes", North East - Organic Division Regional meeting, March 27th 2019, York (YO) United Kingdom.
4. **Pagano A.**, Mazzanti A., Petrillo G., Mancinelli M. "From dinitrobutadienes to dinitroindoles: an original access to vicinal diamines", Ischia Advanced School of Organic Chemistry, September 22nd-25th 2018, Naples (Italy).
5. Bianchi L., Maccagno M., **Pagano A.**, Petrillo G., Tavani C. "Nitrobutadienes as appealing building-blocks in organic synthesis, XXII International Conference on Organic Synthesis, September 16th-21st 2018, Firenze (Italy).
6. Bianchi L., Giorgi G., Maccagno M., **Pagano A.**, Petrillo G., Tavani C. "Polyfunctional indole scaffolds from nitrobutadienes: an original benzannulation onto pyrrole", XII SpanishItalian Symposium on Organic Chemistry, July 2nd-4th 2018, Ferrara (Italy).
7. Bianchi L., Giorgi G., Maccagno M., **Pagano A.**, Petrillo G., Tavani C. "Synthesis of nitrofunctionalized N-heteroaromatic condensed systems", XXVI Congresso Nazionale della Società Chimica Italiana- 10-14 settembre 2017 – Paestum (SA).

### **Honors and Awards**

First Poster Award at XXXIX Convegno Nazionale della Divisione di Chimica Organica della Società Chimica Italiana (September 8th-12th 2019, Torino, Italy) sponsored by EurJOC

### ***Congresses Attended***

1. 10<sup>th</sup> Eurasian Meeting on Heterocyclic Chemistry, September 15th-19th 2019, Milano Marittima (Italy).
2. XXXIX Convegno Nazionale della Divisione di Chimica Organica della Società Chimica Italiana, September 8th-12th 2019, Torino (Italy).
3. North East - Organic Division Regional meeting, March 27th 2019, York (YO) United Kingdom
4. XXII International Conference on Organic Synthesis, September 16th- 21st 2018, Firenze (Italy).
5. XII Spanish-Italian Symposium on Organic Chemistry, July 2nd-4th 2018, Ferrara (Italy).
6. IX Giornate Italo-Francesi di Chimica, April 16th-18th, 2018, Genova (Italy).
7. XVII Merck Young Chemists Symposium, November 13th-15th, 2017, Milano Marittima (Italy)
8. La Giornata della Chimica Ligure, October 20th 2017, Genova (Italy).
9. XXVI Congresso Nazionale Della Società Chimica Italiana- 10-14 settembre 2017 – Paestum (SA).

## ***Courseware***

### ***Courses attended***

#### ***B-type Courses***

1. Fotochimica organica (A. Basso) 2 CFU
2. Progettazione e sviluppo di inibitori di proteina-chinasi come nuovi agenti antitumorali. (S. Schenone) 2 CFU
3. Principal plants in Phytocosmetics and their constituents. (A. Bisio) 2 CFU
4. Innovative pharmaceutical dosage forms: preparation and control methods. (S. Baldassari, G. Caviglioli, B. Parodi, E. Russo) 2 CFU
5. Diversity Oriented Synthesis Of Heterocyclic Compounds. (R. Riva, L. Moni) 2 CFU

#### ***Advanced Courses: A-type courses Given by invited experts***

1. Drug Discovery: Hit to Lead and Lead Optimization- Medicinal Chemistry (Renata Riva, Fabio Bertozzi, Rita Scarpelli, Tiziano Bandiera) (1 credit) - 7/07/2017.
2. Drug Discovery: Hit to Lead and Lead Optimization- Computational Drug Design (Marco De Vivo) (1 credit) - 10/07/2017.
3. Organic Synthesis and Catalysis in the Pharmaceutical Industry (Dr. Paolo Tosatti) (1credit) – 20/09/2019
4. Sustainable electrofuels and chemicals (Prof. Peter Holtappels) (1 credit) – 18/10/2019

#### ***National and International Schools or Workshops***

1. XLIV "A. Corbella" International Summer School on Organic Synthesis, 9th-13th June 2019, Gargnano (BS), Italy
2. Ischia Advanced School of Organic Chemistry, September 22nd-25th 2018, Naples (Italy).
3. XLII International Summer School on Organic Synthesis "A. Corbella" ISOS 2017- Gargnano (Italy), 18-22 June 2017

## **Seminars**

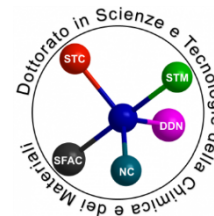
1. 12/06/2017, Dept. of Chemistry and Industrial Chemistry, University of Genova, "Un caso di proficua collaborazione: biocatalisi e prodotti naturali". Dr. Sergio Riva (Istituto di Chimica del Riconoscimento Molecolare, CNR, Milano).
2. 27/10/2017, Dept. of Chemistry and Industrial Chemistry, University of Genova, "Phd students as a bridge between Science and society"
3. 20/12/2017, Dept. of Physics, University of Genova, "Ab Initio Simulations Of Phase-Change Materials". Prof. Riccardo Mazzarello (Institute for Theoretical Solid State Physics and JARA, RWTH Aachen, Germany).
4. 24/01/2018, Dept. of Chemistry and Industrial Chemistry, University of Genova, "Design of magnetic nano-architecture for biomedical applications". Dott. Davide Peddis. 25/01/2018, Dept. of Chemistry and Industrial Chemistry, University of Genova, "Investigation of Biocompatible Gold Supports by means of Reactive Molecular SimulationS". Susanna Monti.
5. 27/02/2018, Dept. of Chemistry and Industrial Chemistry, University of Genova, "Il contributo del DCCI al Programma Nazionale di Ricerche in Antartide". Prof. Marco Grotti e Prof. Paola Rivaro.
6. 03/05/2018, Dept. of Physics, University of Genova, "Elettroni, fotoni e altre particelle: un viaggio nel mondo delle Particelle Fondamentali e delle Onde Gravitazionali", Prof. Luciano Maiani.
7. 04/06/2018, Dept. of Chemistry and Industrial Chemistry, University of Genova, "Targeting the purinergic signaling in the heart New perspectives for understanding the electrophysiological role of adenosine in atrial fibrillation", Dr. Luca Soattin. 17/10/2018 Dept. of Chemistry, University of York, "From idea to Library:the development of 40,000 unique lead-like compounds" - Dr. Pauline Drouhim. 19/10/2018 Dept. of Chemistry, University of York, "Introduction to X-services" - Dr. Adrian Whitwood.
8. 05/09/2019, Dept. of Chemistry and Industrial Chemistry, University of Genova, "Insights in platinum group metal (PGM-free) catalysts for oxygen reduction reaction", Prof. Carlo Santoro.
9. 04/10/2019, Dept. of Chemistry and Industrial Chemistry, University of Genova, "Biocatalysis in medicinal chemistry", Dr. Erica Tassano.
10. 17/10/2019, Pharmacy Dept., University of Genova, "Il paradigma multi-target nel riposizionamento e nella scoperta di sostanze biologicamente attive", Prof. Stefano Alcaro.
11. 22/10/2019 Dept. of Chemistry and Industrial Chemistry, University of Genova, "Molecole in azione: dispositivi e machine molecolari artificiali" Prof. Alberto Credi.
12. 24/10/2019 Dept. of Chemistry and Industrial Chemistry, University of Genova, "Liquid crystal polymers for microrobotics and tissues engineering" Dott. Daniele Martella.
13. 24/10/2019 Dept. of Chemistry and Industrial Chemistry, University of Genova, "Solid State Electrochemistry meets Power2X" Prof. Peter Holtappels

## **Other activities**

- Organizing Committee member of the X Eurasian Meeting on Heterocyclic Chemistry (EAMHC-2019) organized by the Liguria Section of the Società Chimica Italiana (SCI), September 15th-19th, 2019. Milano Marittima-Cervia (Ravenna), Italy. ☐
- Teaching assistance to the module "Organic Chemistry and Laboratory" (Bachelor Degree in Chemistry and Chemical Technologies) academic year 2016/17 and 2017/18 [30 hours each academic year)



**Università degli Studi di Genova**  
**Doctorate in**  
**Sciences and Technologies of**  
**Chemistry and Materials**



**Curriculum: Pharmaceutical, Food and Cosmetic Sciences**

**FRANCESCA PEDRELLI**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*  
**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*  
**Advisor:** Prof.ssa Angela Bisio

**Thesis Title:** Isolation, structural elucidation and evaluation of bioactivity of secondary metabolites from aromatic plants

**Thesis abstract**

Objective of my research project is to identify and isolate new bioactive terpenoids from aromatic plants grown in Liguria. The research work will be developed within the following fields:

- a. Phytochemistry  
The biomass will be extracted with appropriate solvents to yield crude extracts which will be subjected to chromatographic methods (classic methods and HPLC) to obtain purified compounds. Identification and structural elucidation of new compounds will be carried out by spectroscopic (UV, IR, MS, HR-MS 1H- NMR, 13C-NMR) and chromatographic (HPLC-DAD) methods.
- b. Evaluation of the bioactivity of the isolated compounds.  
The crude extracts and the isolated secondary metabolites will then be tested in vitro and/or in vivo for biological activity. Will also be carried out any structural modifications for improving the bioavailability.
- c. Data Analysis  
The obtained data will be evaluated on the basis of classic and advanced statistical methods

**ACTIVITY REPORT**

**Research Activity**

The research activity was mainly carried out at the Department of Pharmacy, University of Genoa, Laboratory of Phytochemistry.

### **Research Period Abroad**

- Stage period at the University of Basel (Department Pharmazeutische Wissenschaften Universität Basel- Pharmazeutische Biologie) from 18/06 to 31/08/18.
- Stage period at the University of Basel (Department Pharmazeutische Wissenschaften Universität Basel- Pharmazeutische Biologie) from 01/06 to 30/06/19.

### **Scientific Publications**

1. Katia Cortese, Silvia Marconi, Carolina D'Alesio, Daniela Calzia, Isabella Panfoli, Sara Tavella, Cinzia Aiello, **Francesca Pedrelli**, Angela Bisio, Patrizio Castagnola. The novel diterpene 7 $\beta$ - acetoxy-20-hydroxy-19,20-epoxyroyleanone from *Salvia corrugata* shows complex cytotoxic activities against human breast epithelial cells. *Life Sciences*. 2019, 232 [116610]
2. Angela Bisio, **Francesca Pedrelli**, Massimiliano D'Ambola, Fabiana Lablanca, Anna Maria Schito, Rafaël Govaerts, Nunziatina De Tommasi, Luigi Milella. Quinone diterpenes from *Salvia* species: chemistry, botany, and biological activity. *Phytochemistry Reviews*. 2019, 18 (3), 665-842

#### *Submitted Publications:*

1. Bisio et al. Antibacterial and ATP synthesis modulating compounds from *Salvia tingitana*. 2019.

### **Communications at Conferences**

#### **Oral communications:**

1. Bisio A., **Pedrelli F.**, De Tommasi N., Schito G.C. et Schito A.M. 2018. Sesterterpenes from *Salvia tingitana* Etl. (Lamiaceae). IX Giornate Italo-Francesi della Chimica- IX Journées Franco-Italiennes de Chimie. Genova 16-18 Aprile.
2. Bisio A., **Pedrelli F.**, De Tommasi N., Schito G.C., Schito A.M. 2018. Antimicrobial Sesterterpenes from *Salvia tingitana* Etl. (Lamiaceae). Scuola "Paolo Ceccherelli - Filiera corta in campo erboristico e medicinale: sviluppo tecnologico e programmazione comunitaria". Albenga 7-9 Giugno.
3. Massimiliano D'Ambola, Soumia Belaabed, **Francesca Pedrelli**, Majed Halawani, Ammar Bader, Roberta Cotugno, Angela Bisio, Nunziatina De Tommasi. CYTOTOXIC LABDANE DITERPENES FROM *PREMNA RESINOSA* (HOCHST.) SCHAUER. XVI Congress of the Italian Society of Phytochemistry jointly 2nd International Congress on Edible, Medicinal and Aromatic Plants (ICEMAP 2019). Alghero 19-21 giugno 2019.

#### **Poster Communications:**

1. Bisio A., **Pedrelli F.**, Dougué Kentsop R. A., Ruffoni B., De Tommasi N., Schito A. M. 2017. Antimicrobial activity of *Salvia Tingitana* Etl. (Lamiaceae), XV Congress of the Italian Society of Phytochemistry jointly with 1<sup>st</sup> International Congress on Edible, Medicinal and Aromatic Plants (ICEMAP 2017), Pisa, 28-30 Giugno 2017.
2. Bisio A., Castagnola P., Panfoli I., Schito A. M., **Pedrelli F.**, De Tommasi N. 2017. Biological activities of extracts and constituents of *Salvia tingitana* Etl. (Lamiaceae), 65th International Congress and Annual Meeting of the Society for Medicinal Plant and Natural Product Research (GA), 3rd to 7th September 2017.

3. Bisio A., **Pedrelli F.**, Dougué Kentsop R. A., Fraternali D., Ruffoni B., De Tommasi N., Schito A. M. 2017, Antibacterial activity of roots of *Salvia corrugata* Vahl, 112° Congresso della Società Botanica Italiana; IV International Plant Science Conference (IPSC), Parma 20-22 Settembre 2017.
4. Bisio A., Pessa L., **Pedrelli F.**, De Tommasi N. and Giacomini M. From the experience of “PLANT” and “PYRGY” EU Projects onwards: interdisciplinary link of medicinal plant science with history and art. Botany at the intersection of Nature, Culture, Art and Science. Sicilia 28-30 giugno 2018.
5. Panfoli I., D. Calzia, Esposito A., P. Degan, A. Bisio, *Pedrelli F.*, Schito C, E. Traverso, Modulation of oxidative stress in the rod outer segment aerobic metabolism by diterpene manool and sclareol extracted from *Salvia tingitana*. EVER Congress. Nizza 4-6 ottobre 2018.
6. Bisio A., **Pedrelli F.**, Panfoli I., Calzia D., De Tommasi N., Schito G. C., Schito, Annamaria, Antimicrobial and ATP synthase modulating activity of the surface constituents of *Salvia tingitana* Etl. (Lamiaceae), 113° Congresso della Società Botanica Italiana, Fisciano (SA), 12-14 settembre 2018.
7. E. Lazarova, L. Pastorino, **F. Pedrelli**, A. Bisio, M. Giacomini. A New Technological Tool to Manage Edible Flowers for Health Purposes: the Interreg Alcotra ANTEA project. Buenos Aires, Argentina; March 26–31, 2019.
8. Roméo Arago Dougué Kentsop, Elena Lazarova, **Francesca Pedrelli**, Marco Savona, Martina Fabiano, Mauro Giacomini, Barbara Ruffoni, Anna Maria Schito, Nunziatina De Tommasi, Angela Bisio, Establishment of hairy root cultures of *Salvia corrugata* Vahl, XVI Congress of the Italian Society of Phytochemistry jointly with 2nd International Congress on Edible, Medicinal and Aromatic Plants (ICEMAP 2019). Alghero 19-21 giugno 2019.
9. Silvia Sillano, Vincenzo Minganti, **Francesca Pedrelli**, Angela Bisio, Giuliana Drava. Trace elements in edible flowers from Liguria: an exploratory study, XVI Congress of the Italian Society of Phytochemistry jointly with 2nd International Congress on Edible, Medicinal and Aromatic Plants (ICEMAP 2019), Alghero 19-21 giugno 2019.
10. Angela Bisio, **Francesca Pedrelli**, Martina Fabiano, Roméo Arago Dougué Kentsop, Gian Carlo Schito, Anna Maria Schito, Nunziatina De Tommasi, Abietane Diterpene constituents from the roots of *Salvia tingitana* Etl. (Lamiaceae), “114° Congresso della Società Botanica Italiana (VI International Plant Science Conference)”. Padova, 4-7 settembre 2019.
11. Angela Bisio, **Francesca Pedrelli**, Roméo Arago Dougué Kentsop, Massimiliano D’Ambola, Martina Fabiano, Barbara Ruffoni, Gabriella Piatti, Gian Carlo Schito, Nunziatina De Tommasi, Anna Maria Schito, Antibacterial activity of abietane diterpenes from the roots and hairy roots of *Salvia corrugata* Vahl, 67th International Congress and Annual Meeting of the Society for Medicinal Plant and Natural, Innsbruck, Austria, 1-5 settembre 2019.

### **Congresses Attended**

1. “XV Congress of the Italian Society of Phytochemistry jointly with 1st International Congress on Edible, Medicinal and Aromatic Plants (ICEMAP 2017)”, Pisa, 28-30 giugno 2017.
2. “65th International Congress and Annual Meeting of the Society for Medicinal Plant and Natural Product Research (GA)”, 3rd to 7th September 2017.
3. “112° Congresso della Società Botanica Italiana; IV International Plant Science Conference (IPSC)”, Parma 20-22 settembre 2017.
4. “IX Giornate Italo-Francesi della Chimica- IX Journées Franco-Italiennes de Chimie”. Genova 16-18 Aprile 2018.



5. Bisio A., Pessa L., Pedrelli F., De Tommasi N. and Giacomini M. From the experience of "PLANT" and "PYRGY" EU Projects onwards: interdisciplinary link of medicinal plant science with history and art. Botany at the intersection of Nature, Culture, Art and Science. Sicilia 28-30 giugno 2018.
6. Panfoli I., D. Calzia, Esposito A., P. Degan, A. Bisio, Pedrelli F., Schito C, E. Traverso. Modulation of oxidative stress in the rod outer segment aerobic metabolism by diterpene manool and sclareol extracted from *Salvia tingitana*. EVER Congress. Nizza 4-6 ottobre 2018.
7. Bisio A., Pedrelli F., Panfoli I., Calzia D., De Tommasi N., Schito G.C., Schito, Annamaria. Antimicrobial and ATP synthase modulating activity of the surface constituents of *Salvia tingitana* Etl. (Lamiaceae). 113° Congresso della Società Botanica Italiana, Fisciano (SA), 12-14 settembre 2018.
8. Swiss Pharma Science Day 2018, Bern, 22 Agosto 2018.
9. Meeting di progetto ANTEA, ALCOTRA. 27 marzo 2019, Savona.
10. Meeting di progetto INNOV. 3 Aprile 2019, Nizza. XVI Congress of the Italian Society of Phytochemistry jointly with 2nd International Congress on Edible,
11. Medicinal and Aromatic Plants (ICEMAP 2019). Alghero 19-21 giugno 2019.
12. "67th International Congress and Annual Meeting of the Society for Medicinal Plant and Natural". Innsbruck, Austria, 1-5 settembre 2019
13. 114° Congresso della Società Botanica Italiana (VI International Plant Science Conference)". Padova, 4-7 settembre 2019.

## **Courseware**

### ***Courses attended and passed***

#### ***Courses Given by Teachers of Unige and IIT:***

1. "Nomenclatura INN ed IUPAC di farmaci a struttura organica" Prof. G.Grossi (DIFAR) (2 credits)
2. "Progettazione e sviluppo di inibitori di proteina chinasi come nuovi agenti antitumorali" Prof.ssa S. Schenone (DIFAR) (2 credits)
3. "Metodi fisici in chimica organica" (corso di tipo F) Prof. Lucchesini (DIFAR) (7 credits).
4. "Ricerca bibliografica e brevettuale nelle scienze farmaceutiche tramite banche". Prof.ssa C. Brullo e Prof.ssa P. Fossa (DIFAR) (2credits).
5. "Principali piante utilizzate in Fitocosmesi e loro costituenti". Prof.ssa A. Bisio (DIFAR) (2credits).
6. "Tecniche strumentali per la determinazione di elementi in traccia di interesse farmaceutico, alimentare, ambientale". Prof V. Minganti e Prof.ssa G. Drava (DIFAR) (2 credits).

#### ***Courses Given by invited experts:***

1. "Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials; Novel Materials for energy storage and conversion", Prof. Dr. Thomas Fassler
2. "An introduction to nanoscale magnetism for biomedical applications", Dr. Neil Telling
3. "Superhard materials: structural chemistry of boron and borides", Prof. Peter Rogl

### ***National and International Schools or Workshops***

1. Workshop: "Una rosa, è una rosa, è una rosa" (Gertrude Stein). Incontro tra scienza, arte e territorio. Genova, Palazzo Ducale, Sala del Minor Consiglio, 26 maggio 2017
2. Workshop: "The Nagoya Protocol: access and benefit-sharing of nature's genetic resources". Firenze, 27 Febbraio 2017, Rettorato dell'Università di Firenze, Piazza San Marco 4
3. Scuola "Paolo Ceccherelli - Filiera corta in campo erboristico e medicinale: sviluppo tecnologico e programmazione comunitaria". Albenga 7-9 Giugno 2018.

### ***Seminars Attended***

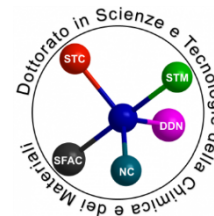
1. "Il marketing cosmetico: dalla mission aziendale alla risposta del consumatore", Dr.ssa Silvia Rum (DIFAR)
2. "Odori, profumi e feromoni come mediatori chimici olfattivi", Dr.ssa Chiara Lacapra (DIFAR)
3. "Giocare sporco: PAINS e composti promiscui", Dr.ssa Anita Parricchi (DIFAR)
4. "Tubercolosi ed altre patologie polmonari: stato dell'arte e recenti sviluppi terapeutici", Dr.ssa Elda Meta (DIFAR)
5. "Problematiche relative alla qualità e sicurezza delle materie prime e degli eccipienti. Tracciabilità e provenienza", Dr. Piero Iamartino
6. "Chemical biology and medicinal chemistry of human proteasomes", Prof. Herman Overkleeft
7. "Patient Safety Centre di Lipsia: una iniziativa interdisciplinare per la sicurezza del paziente", Dott. Roberto Frontini
8. "Cancer Tissue Engineering: new technological approaches for providing alternative 3-dimensional in vitro tumor models for cancer biology and drug testing", Dr.ssa Silvia Scaglione
9. "Le farmaci proteici e le grandi rivoluzioni della terapia", Dr. Cantelli Forti
10. "I vaccini: dalle origini ai giorni nostri (the vaccines: from the origins to the present day)", Dott.ssa Sanna Monica (DIFAR)
11. "Chronic Obstructive Pulmonary Disease (COPD): a pathology overview and the possible effects of Particulate Matter (PM)" (DIFAR), Dott. Brignole Daniele (DIFAR)
12. "Imaging in Oncology", Dott.ssa Pastorino Sara (DIFAR)
13. "Depression: new therapeutic strategies", Dott. Sadeghi Mohamed (DIFAR)
14. "Probiotics: properties, uses and interaction with human gut microbiome", Dott.ssa Turrini Federica, (DIFAR)
15. "Epigenetics changes, trace elements and antioxidant status for cancer prevention", Prof. Barbara Anna Bobrowska-Korczak (DIFAR)
16. "Chemistry in the kitchen from traditional to molecular cooking" Dott.ssa Ilaria Giacchello (DIFAR)
17. "Oral diseases and their treatment: an overview" Dott. Kartik Neduri (DIFAR)
18. "Five isoforms of N, N, N-tris(tert-butoxycarbonyl)-L-arginine depending on procedure and the investigation of their reactivity in esterification reactions" Dott. Gaby Brice Taptue (DIFAR)
19. "Deubiquitinase inhibition as therapeutic strategy", Dott.ssa Vittoria Zoppi (DIFAR)
20. "Astrochemistry: the chemistry of stars" Dott.ssa Valeria Francesconi (DIFAR)
21. "Preliminary in vitro assays to evaluate anticancer drugs" Dott.ssa Chiara Greco (DIFAR)
22. "Design of experiment: full factorial design and case study" Dott.ssa Mariam Hooshyari (DIFAR)
23. "Production of biopharmaceutical proteins: particular case of the plants" Dott. Romeo Arago Dougue Kentsop (DIFAR)

### ***Other Activities***

1. Segreteria organizzativa al Workshop: “Una rosa, è una rosa, è una rosa” (Gertrude Stein). Incontro tra scienza, arte e territorio. Genova, Palazzo Ducale, Sala del Minor Consiglio, 26 maggio 2017.
2. Attività di supporto alla didattica nell’ambito del Corso di Tecnologia, Socioeconomia e Legislazione Farmaceutica I per Farmacia (30 ore), AA 2017-2018, primo semestre.
3. Attività di supporto alla didattica nell’ambito del Corso di Analisi dei Farmaci II per Farmacia (30 ore), AA 2017-2018, primo semestre.
4. Segreteria scientifica alla Scuola “Paolo Ceccherelli – Filiera corta in campo erboristico e medicinale: sviluppo tecnologico e programmazione comunitaria”, Albenga 7-9 giugno 2018.
5. Attività di supporto alla didattica nell’ambito del Corso di Sintesi dei Farmaci per CTF (60 ore), AA 2018- 2019, primo semestre.
6. Corso: “Ottimizzazione delle variabili cromatografiche in HPLC e UHPLC”, Milano, Hotel Berna. 14 maggio 2019.



**Università degli Studi di Genova**  
**Doctorate in**  
**Sciences and Technologies of**  
**Chemistry and Materials**



**Curriculum: Science and Technology of Materials**

**ALEJANDRO PLAZA**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2015*

**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*

**Advisor:** Prof. Daniele Marré

**Thesis Title:** Fabrication and characterization of bidimensional electronic gas (2DEG) in ZnO based heterostructures

**Thesis abstract**

The complex nature of oxides and its interfaces induces complex behaviours that make them a strong platform to produce advanced and innovative nanodevices. ZnO is one of the most promising transition metal oxides with many useful properties, like piezoelectricity, large exciton binding energy, is an eco-friendly material, low cost, wide band gap, transparency, potential sensor uses, etc.

Samples of ZnO films and heterostructures were produced on three different substrates: SrTiO<sub>3</sub> 110 (STO), Sapphire 001 and ZnO 001. Two routes were employed for the deposition of the samples. A first reference set of Co doped ZnO heterostructures were produced by Pulsed Laser Deposition (PLD) on top of STO substrates with the objective of studying magnetoresistance modulation by means of electric field. A second set of heterostructures of ZnO were also produced by PLD on top of ZnO substrates with the objective of studying effective mass dependence on applied magnetic field. Finally, a more difficult route of fabrication by Molecular Beam Epitaxy (MBE) was tackled with the aim of producing higher quality ZnO films and heterostructures in order to enlarge the breath and depth of previous studies.

The samples were characterized by Reflection High Energy Electron Diffraction (RHEED), Scanning Electron Microscopy (SEM-EDS), Atomic Force Microscopy (AFM), X-ray diffraction (XRD) and Reflectivity (XRR), Electric Transport Measurement (PPMS).

The analysis of PLD Co doped ZnO/STO heterostructures, showed a negative dependence of magnetoresistance on carrier charge density. This effect was interpreted in terms of the bounded polaron model (BPM) in which the charge carrier density modifies the average polaron size but not its number. This study sheds light on the nature of TM doped ZnO as a polaron mediated superparamagnet, rather than a Diluted Magnetic Semiconductor (DMS).

The analysis of PLD Mg doped ZnO heterostructures on ZnO, showed a positive dependence of effective mass on magnetic field intensity. Some possible mechanisms potentially responsible for this

behavior were analyzed and an explanatory hypothesis was advanced based in band non parabolicity and electron interactions.

A significant number of trials (142) were carried out to produce ZnO films and heterostructures by MBE under low deposition rate, mild oxidizing conditions and high misfit substrate (sapphire). The structural and morphological characterization of the samples by RHEED, AFM, XRD, XRR and SEM- EDS resulted in an exploration of the parameter space that entitled us to shed light in some specific details of the film growth under the given conditions and to suggest a growth mechanism.

## ACTIVITY REPORT

### *Research Activity*

The research was mainly carried out at the Department of Physics of the University of Genova

#### *Scientific Publications*

1. Effect of free charge carrier density on magnetic behavior of (Zn,Co)O thin film studied by Field Effect modulation of magnetotransport properties; Bellingeri, Rusponi, Lehnert, Brune, Nolting, **Plaza**, Marré accepted to Scientific Reports and available on line at: <https://www.nature.com/articles/s41598-018-36336-w>
2. Investigation of the effective mass enhancement in ZnO/ZnMgO heterostructures through quantum effects; Leveratto, Pallecchi, Timossi, **Plaza**, Zeitler, Jost, Bellingeri, Marré submitted to Scientific Reports

#### *National and International Schools and Workshops*

1. 17/02/2016, Dept. of Chemistry and Industrial Chemistry, "IWIW 2016 - International Workshop on Industrial Waste Approaches and Technologies for the Recovery of Raw Materials by Complex Products End of Life", Genoa, Italy.
2. 13/10/2016, University of Pavia - Ph.D. School of Electrical and Electronics Engineering and Computer Science, "Metamaterials and their applications in acoustics, microwaves and optics", Prof. Alessandro Toscano, Department of Engineering, University of Roma Tre.
3. 12/01-14/1/2017, International Centre for Theoretical Physics, "18th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods", Miramare, Trieste, Italy
4. 11/04/2017-21/4/2017, "International School of Oxide Electronics" (ISOE2017), Cargèse, Corsica, Francia
5. 7/11/2017, SMARTcup Liguria 2017, "Business Make Up - Posizionamento dell'azienda sul mercato e sui social network", Sara di Paolo e Lorenzo Novaro, Genova, Italy
6. 08/10/2018, Dept. of Physics & CNR-SPIN, "Workshop on Microactuators", UniGe, Genoa, Italy

#### *Meetings*

1. 19/06/2017, CNR-SPIN – "Spin progetta il suo futuro", Federghini, Spin Genova, Italia

2. 23/06/2017, Dept. of Chemistry, "Il dottorato in chimica: dove siamo e dove vogliamo arrivare", Dipartimento di Chimica "Giacomo Ciamician", Dipartimento di Chimica Industriale "Toso Montanari", Alma Mater Studiorum-Università di Bologna.

### ***Conferences attended***

1. 19-21/09/2016, SuperFOx 2016, "Third Conference on Superconductivity and Functional Oxides", Department of Applied Science and Technology (DISAT), Politecnico di Torino.
2. 20/09/2017, University of Pavia – Sheet resistance and resistivity measurements of thin conducting, semiconducting and superconducting films", J. Krupka, IMWS-AMP 2017, University of Pavia

## ***Courseware***

### ***Courses attended and passed***

#### ***Courses Given by Teachers of the UniGe & IIT***

1. Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations" Dott. Luca de Trizio, Istituto Italiano di Tecnologia, (1 credit)
2. Science and technology of 2D crystals, Prof. Francesco Bonaccorso, Istituto Italiano di Tecnologia, Italy (1 credit)
3. Synthesis, structure and functional properties of intermetallic compounds, Prof.ssa. Adriana Saccone, Dip. of Chemistry & Industrial Chemistry (2 credits)
4. Mathematical Methods for Chemistry, Prof. Ottinelli (2 credits)
5. Advanced Crystallography, Prof. Martinelli (4 credits)
6. Surface Science, Prof. Vattuone (2 credits)
7. Introduction to functional ceramic materials, Prof. Buscaglia (2 credits)
8. Basic Scanning and Transmission Electron Microscopies, Prof.ssa. Riani (3 credits)

#### ***Courses Given by invited experts:***

1. 17 e 18/02/2016, Dept. of Chemistry and Industrial Chemistry, "Low and Very Low Temperatures: Methods of Producing and Measuring Cryogenic Temperatures", Ivan Čurlík, Department of Physics, Mathematics and Technics, University of Prešov, Slovakia (1 credit)
2. 29/02/2016, Dept. of Farmacy - DIFAR – Medicine and cosmetic product Chemistry, "NIR spectroscopy: theory and applications", Tiziana Cattaneo e Roberto Giangiacomo, CRA-IAA (Consiglio per la Ricerca in agricoltura e l'analisi dell'economia agraria) Unità di ricerca per i processi dell'industria agro-alimentare Ingegneria e Trasformazioni agroalimentari, Milan, Italy (1 credit)
3. 5 e 6/4/2016, Dept. of Chemistry and Industrial Chemistry, "Physics in extreme conditions", Prof. RNDr. Marian Reiffers, DrSc., FInstP. Faculty of Humanities and Natural Sciences, University of Presov, Slovakia
4. 22/04/2016, Dept. of Chemistry and Industrial Chemistry, "Design of magnetic nano-architecture", Dott. Davide Peddis, Istituto di Struttura della Materia, CNR – Roma (1 credit)

5. 14 e 16/06/2016, Dept. of Chemistry and Industrial Chemistry, "Advanced Materials for Renewable Energy (Energy Saving)", Prof. Peter Rogl, Institute of Physical Chemistry, University of Vienna, Austria (1 credit)
6. 5-7/12/2016, CINECA, "Material science codes on innovative HPC architectures", CINECA, Bologna, Italia (3 days)
7. 6 e 7/06/2017, Dept. of Chemistry and Industrial Chemistry, "Superhard materials: structural chemistry of boron and borides", Prof. Peter Rogl, Institute of Physical Chemistry, University of Vienna, Austria

### **Seminars**

1. 22/01/2016, Dept. Of Physics, "Nanostructured inks for advanced devices: from research to business", Alessandro Chiolerio & Sergio Bocchini, Istituto Italiano di Tecnologia, Center for Space Human Robotics, Torino, Italy
2. 1/03/2016, Dept. Of Physics, "From thermal rectifiers to thermoelectric devices", Prof. Giuliano Benenti, Università degli Studi dell'Insubria, Italy.
3. 17/03/2016, Dept. of Physics, "Discussion on thermoelectric properties of Iron based materials", Dr. Marcin Matusiak, Institute of Low Temperature & Structure Research, Polish Academy of Sciences, Wroclaw, Poland
4. 17/03/2016, Dept. of Physics, "The thermal Hall effect, transverse thermal conductivity and Righi-Leduc effect in unconventional superconductors", Dr. Marcin Matusiak, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wroclaw, Poland
5. 18/04/2016, Dept. of Physics, "Transport properties of nanostructured graphene", Prof. Antti-Pekka Jauho, Center for Nanostructured Graphene (CNG), DTU Nanotech, DTU (Technical University of Denmark)
6. 21/04/2016, Dept. of Physics, "Surface chemical reactions at epitaxial graphene and materials 'beyond graphene' ", Prof. Politano, University of Calabria, Department of Physics
7. 27/04/2016, Dept. of Physics, "Coarse-grained modelling of large biomolecular systems", Dott. Paolo Mereghetti, Istituto Italiano di Tecnologia, Center for Nanotechnology Innovation, Pisa, Italy
8. 5/05/2016, Dept. of Chemistry and Industrial Chemistry, "Aspetti e prospettive della moderna industria siderurgica", Ing. Franco Belgrano, Isosistemi s.r.l.
9. 11/07/2016, Dept. of Physics, "Towards an atomic scale technology: electronics mechanics with single molecules", Dott.Prof.ssa Francesca Moresco, Institute for Materials Science della Technische Universität di Dresda.
10. 22/09/2016, Dept. of Physics, "Conformal QED in two-dimensional topological insulators", Dott. Giandomenico Palumbo, Dipartimento di Fisica, Università di Utrecht.
11. 13/10/2016, University of Pavia-Ph.D. School of Electrical and Electronics Engineering and Computer Science, "Metamaterials and their applications in acoustics, microwaves and optics", Prof. Alessandro Toscano, Department of Engineering, University of Roma Tre.
12. 17/11/2016, University of Pavia – Dept. of Physics, "Physics in the Brain", Prof. Egidio D'Angelo, Dipartimento di Scienze del Sistema Nervoso e del Comportamento, Università di Pavia
13. 21/11/2016, Dept. of Physics, "Exploring the transformation mechanisms of matter at the nanoscale with computer simulations", Dott. Fabio Pietrucci, Sorbonne Universités – Université Pierre et Marie Curie
14. 16/01/2017, University of Pavia - Ph.D. School of Electrical and Electronics Engineering and Computer Science, "Smart devices for electrical power systems", Prof. Alessandro Lidozzi, Centre for Power Electronics and Drivers Department of Engineering, University of Roma Tre.

15. 03/02/2017, Dept. of Physics, "Sviluppo di nuovi materiali per olografia: dalla molecola al materiale", Dott. Andrea Bianco, Istituto Nazionale di Astrofisica, Osservatorio di Brera.
16. 07/02/2017, Dept. of Physics, "On the optical absorption of intermediate band semiconducting nanoparticles", R. Gaspari, Istituto Italiano di Tecnologia.
17. 11/05/2017, Dept. of Physics, "Tailoring nanostructures by supersonic cluster beam deposition and non-thermal laser ablation", L. Gavioli, Università Cattolica del Sacro Cuore.
18. 31/05/2017, Dept. of Physics, "La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> thin films for sensing applications", Dott. Laurence Méchin, Groupe de recherche en Informatique, Image, Automatique et Instrumentation de Caen Normandie Univ, UNICAEN, ENSICAEN, CNRS, GREYC.
19. 25/10/2017, CNR-SPIN – "Critical current density in NbTi & MgB<sub>2</sub> wires, FeSe and Ba(Fe<sub>0.92</sub>Co<sub>0.08</sub>)<sub>2</sub> As<sub>2</sub> bulks", D. Gajda, Institute of low temperature and Structure Research Wroclaw, Poland
20. 14/11/2017, University of Pavia – "3D Scaffolds Cellularised with Human Vascular Cells for Complex Culture and Maturation in Bioreactors: Applications in Regenerative Medicine and Beyond", Professore Diego Mantovani, Professore Ordinario all'Università di Laval in Quebec, Canada.
21. 15/11/2017, Dept. of Physics, "Field Theory Description of Topological States of Matter", Dr. Andrea Cappelli, INFN Firenze.
22. 24/11/2017, University of Genova, Dept. of Chemistry and Built Environment (DICCA), "The Generation of Stress and Fracture in the Storage Particles of Lithium-Ion Batteries", Prof. Robert Mc Meeking, mechanical Engineering School, University of California Santa Barbara
23. 6/12/2017, University of Genova, Dept. of Chemistry and Industrial Chemistry, "Effect of isotactic polypropylene microstructure on crystallization and properties: the role of regiodefects", Davide Tranchida, Ph.D. (Borealis Polyolefine GmbH)
24. 6/12/2017, Dept. of Physics, "Computational protocols to investigate nucleation and growth at hybrid systems interfaces", Giovanni Barcaro CNR-IPCF, National Research Council—Institute of Chemical and Physical Processes, Pisa, Italy.
25. 20/12/2017, CNR-SPIN - University of Genova, Dept. of Physics, "Ab Initio Simulations of Phase-Change Materials", Riccardo Mazzarello, Institute for Theoretical Solid State Physics and JARA, RWTH Aachen, Germany
26. 25/01/2018, University of Pavia – Dept. of Physics, "Nanotechnology at work: how to marry an academic career with entrepreneurship", Prof. Paolo Milani, Dipartimento di Fisica and CIMAINA (Centro Interdisciplinare Materiali e Interfacce Nanostrutturati), Università di Milano
27. 10/05/2018, Dept. of Physics, "Biomimetic Complex Systems for Soft Actuation and Neural Computing", Prof. Paolo Milani, Dipartimento di Fisica and CIMAINA (Centro Interdisciplinare Materiali e Interfacce Nanostrutturati), Università di Milano
28. 11/05/2018, Dept. of Physics, "Nano- and Micro-manufacturing with nanoparticles produced in the gas phase for function and length scale integration", Prof. Paolo Milani, Dipartimento di Fisica and CIMAINA (Centro Interdisciplinare Materiali e Interfacce Nanostrutturati), Università di Milano
29. 10/9/2018, Dept. of Physics, "Quantum thermodynamics in strongly coupled quantum dots", Prof. Dr. Thomas Schmidt, Faculté des Sciences de la Technologie et de la Communication Physique et Matériaux Université du Luxembourg.
30. 26/09/2018, University of Pavia - Ph.D. School of Electrical and Electronics Engineering and Computer Science, "Quality and Operations Management in R&D", Alan Franzi & Alessandro Schito, Facoltà di Ingegneria, Università di Pavia.

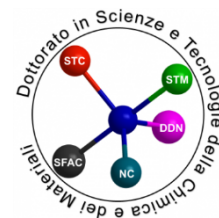


***Other Activities***

1. Tutor of OFA, Matematics, UniGe. Sept-Oct.2016
2. Tutor of OFA, Matematics, UniGe. Oct.2017-Aug.2018
3. Tutor of Mathematics & Physics, Engineering School, UniGe, From Aug. 2018
4. Tutor of Mathematics, UniGe, From Sept. 2019



**Università degli Studi di Genova**  
**Doctorate in**  
**Sciences and Technologies of**  
**Chemistry and Materials**



**Curriculum: NanochemistryY**

**IRENE ROSINA**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*  
**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*  
**Advisors:** Prof. Liberato Manna (IIT), Dr. Luca De Trizio (IIT), Prof. Paola Riani (Unige)

**Thesis Title:** Exploiting Cation Exchange Reactions in Doped Colloidal Adamantic Semiconductor Nanocrystals: from synthesis to applications

**Thesis abstract**

Colloidal quantum dots (CQDs) have tunable optical transition through manipulation of nanocrystal size, shape and surface. Among luminescent materials, near-infrared (NIR) active semiconductors are of particular interest since they can be used in several applications, from the labeling in living tissues, to the integration in commercial optoelectronic devices, like photovoltaics for solar energy conversion or photodetectors from visible to the near-infrared and mid-infrared. Among the benefits provided by NCs semiconductor, parameters like the color of emission, the emission band, the stability, can be tuned as a function of the size of the crystal.

In addition, the exciting promise of CQDs is the associated easy and low-cost device fabrication process. In fact, solution-based techniques like spin-coating, dip coating and inkjet printing are typically used. In this thesis I proposed to exploit cation exchange (CE) reactions as a convenient tool to finely transform colloidal nanocrystals (NCs) directly in solution or deposited as NC films. These reactions allow to substitute a fraction or all “host” metal cations of pre-synthesized NCs with new “guest” cations while preserving both NCs’ size, shape and, typically, crystal structure. Depending on the miscibility of the reactant and product materials, and on the kinetics of the CE reaction, different types of nanostructures can be accessed ranging from alloy NCs, doped systems, dimers, core@shell (or core@graded-shell) heterostructures even with elaborated architectures (i.e., quantum wells, multiple-cores@shell).

We developed in this way, metastable nanoheterostructures (NHCs) to control the NCs optoelectronic properties in the NIR. This study provides an overview of the CE on adamantic semiconductors NCs, in particular on II-VI, I-III-VI<sub>2</sub> and III-VI compounds. We first explore cadmium chalcogenides mercury exchange NCs as Cd<sub>1-x</sub>Hg<sub>x</sub>Te CQDs which have been widely studied for the NIR photodetectors and photovoltaic devices. Our synthesis method takes part of a wide systematic investigation process, by varying specific physical parameters, such as the reaction temperature and the molar ratio. More

specifically, it is demonstrated that the characterization of the process is mainly influenced by the amount and concentration of solvents/precursors ratio. All these aspects were studied to have control on the size, shape, surface composition and crystalline phase after mild conditions of annealing into stable connected crystals. This peculiarity could be exploited to boost the photogenerated charges diffusion in polycrystalline photoconducting films fabricated by means of an ink of NCs solution. Additionally, another aspect studied was the ligand-shell stabilizing the colloidal NCs, which constrains the charge transfer efficiency among the nanocrystals. Indeed, despite the ligand exchange and stripping chemistries have been widely used, their basic mechanistic are still to the beginning and some nanocrystals are not prone to the ligand removal. Moreover, they may exhibit colloidal instabilities if the exposed metal cations desorb from the surface during the stripping. Instead, our NHCs enables to avoid the post-process ligand stripping and nonetheless, the final annealing step can be performed in milder conditions.

The carrier transport in QD devices differs fundamentally from band transport in bulk semiconductors. One clear direction to bring these QDs devices toward practical relevance is to improve the high charge mobility of the photogenerated charges. Noteworthy, the granularity of the system and the consequent coupling between adjacent dots can produce additional physical parameters, like charge recombinations and losses. Moreover, the carrier diffusion length can be limited by trapping sites<sup>4</sup>. To overcome these limitations, post- synthetic strategies that couple the high quality NCs solutions with ideal properties (band gap, absorption, monodispersivity) and high quality, films (quantum dot packing, passivation, and absorptive/conductive properties) are necessary. Above these considerations, CE can be exploited to addresses NCs solution through surface uniformity from the nano- to the macroscopic scale.

This is the first step toward electronic coupling between the separate building blocks of nanocrystals.

In the last part, results about other NIR emitters we studied are reported. In particular III-V Indium Phosphide (InP) NCs were used as host lattices to combine their narrow emission luminescence with that of rare earth phosphors, like Lanthanides, to improve the emission performances. Afterwards we describe also I-III-VI<sub>2</sub> system as CuInS<sub>2</sub> photoluminescence modulation study has reported varying their preheating time

## **ACTIVITY REPORT**

### ***Research Activity***

#### ***Communications at Conferences***

##### ***Poster communications***

1. E-MRS Fall 2018 in Warsaw University of Technolog

### ***Courseware***

#### ***Courses attended and passed***

##### ***Courses Given by Teachers of the Unige and IIT (B type course)***

1. Nanochemistry School Module 1 Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations (1 credit). Speaker: Luca de Trizio

2. Nanochemistry School Module 2. Basics of Crystallography and Diffraction by crystals (1 credit) .  
Speaker: Mirko Prato
3. Nanochemistry School Module 3 Introduction to electron microscopy. (1 credit) Speakers: R. Brescia, R. Marotta, Z. Dang, J. Buha
4. Nanochemistry School Module 4 Opto-Electronic Properties of Semiconductor Quantum Dots. (1 credit) Speaker: Iwan Moreels
5. Nanochemistry School Module 5. "Spectroscopies for chemical analysis" (1 credit) Speakers: Francisco Palazon, Roman Krahne, Iwan Moreels
6. Nanochemistry School- module 6. "Mechanical properties + atomic force microscopy" (1 credit)  
Speaker: Luca Ceseracciu, Marco Salerno
7. Nanochemistry School- module 7. "Water transfer nanoparticles" (1 credit) Speaker: Teresa Pellegrino
8. Nanochemistry School Optical Spectroscopy of Colloidal Nanocrystals (1 credit) Speaker: Dmitry Baranov.
9. Optical properties of low-dimensional materials (1 credit) Speaker: Ilka Kriegel

***Courses Given by invited experts (A Type course):***

1. Nanoparticle Chemistry for the use of Energy Conversion and Theranostics, Prof. Clemens Burda from Case Western Reserve University in Cleveland, OHIO, USA
2. Scientific Communication skills, Dr. Roman Krahne, IIT
3. 'X-ray Microscopies, Prof. Cinzia Giannini - Institute of Crystallography – National Research Council Bari Italy

***Seminars:***

1. Synthetic methodology for colloidal synthesis of Nanomaterials: Challenges and opportunities.  
Speaker D. Talapin
2. High-Throughput design of doped colloidal nanocrystals. Speaker: Emory Chan
3. Perovskite Nanocrystals: the new generation of defect tolerant luminescent material. Speaker: Sameer Sapea
4. Standardization methods for the synthesis of single-core and multi-core magnetic nanoparticles for medical applications. Speaker: Helena Gavilan Rubio; 2<sup>nd</sup> October 2017
5. Aberration-corrected STEM: sub-Å resolution imaging, atomic-resolution elemental mapping, and vibrational spectroscopy. Speaker: Ondrej L. Krivanek; 4<sup>th</sup> October 2017
6. Interface engineering for efficient and stable organic and perovskites semiconductors. Speaker: Prof. Kymakis, 14<sup>th</sup> November 2017
7. Flat Optics Based on Metasurfaces. Speaker: Prof. Federico Capasso, John A. Paulson School of Engineering and Applied Sciences, Harvard University, USA; 13<sup>th</sup> December 2017
8. The physics of the Universe, over more than 60 orders of magnitude of length. Speaker: Prof. Dr. Antonio Ereditato, Director - Albert Einstein Center for Fundamental Physics, Laboratory for High Energy Physics, University of Bern; 18<sup>th</sup> December 2017
9. One-year stable perovskite Solar Cells by 2D-3D interface engineers. Speaker: Giulia Grancini – EPFL; 2<sup>nd</sup> February 2018
10. Membrane Engineering. Speaker: Prof. Enrico Drioli, National Research Council - Institute on Membrane Technology (ITM–CNR) & University of Calabria - Department of Environmental Engineering and Chemical Engineering; 5<sup>th</sup> February 2018

11. Colloidal semiconductor nanocrystals. Speaker: Dr. Ivan Infante, Vrije Universiteit, Amsterdam; 26th February 2018
12. "Photophysics and photonic applications of alternative plasmonic nanomaterials" speaker: Francesco Scotognella from Dipartimento di Fisica, Politecnico di Milano; 5<sup>th</sup> April 2018
13. "Quantum optics with two-dimensional materials: from many-body physics to quantum information" speaker: Francesco Scotognella from Dipartimento di Fisica, Politecnico di Milano; 5<sup>th</sup> April 2018
14. "Lab-in-a-Fiber Photonic Devices" speaker: Stavros Pissadakis, Institute of Electronic Structure and Laser (IESL) & Foundation for Research and Technology - Hellas (FORTH); 21<sup>st</sup> May 2018
15. "Designing and Studying Perovskite Materials for a Renewable Energy Future", Prof. Clemens Burda - Department of Chemistry, Case Western Reserve University, 5<sup>th</sup> June 2018
16. Nanochemistry Seminar: "Attosecond microscopy and control of matter down to the nucleus" speaker: Fabrizio Carbone from Laboratory for ultrafast microscopy and electron scattering (LUMES); 19<sup>th</sup> October 2018 Faculty of Basic Sciences, Institute of Physics (IPhys) and École Polytechnique Fédérale de Lausanne (EPFL)
17. Nanochemistry Seminar – Title: "Colloidal Copper Chalcogenide Nanocrystals: a Versatile New Class of Optoelectronic Materials" ,Dr. Chenghui Xia - Utrecht University, Debye Institute for Nanomaterials Science
18. "Optoelectronics Seminar – Novel plasmonic and photonic nanomaterials for optoelectronic and bio applications", Dr. Gleb Tselikov, Laboratory Lp3- CNRS, France

### ***National and International Schools or Workshops***

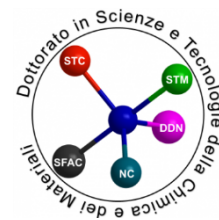
1. International Summer School on Photovoltaics and New Concepts of Quantum Solar Energy Conversion- QuantSol2019 – 1-8 September 2019 in Hirschegg, Austria
2. ETSF- 24th Workshop on Electronic Excitations- Light-matter interactions and optical spectroscopy from infrared to X-rays- 16-20 September 2019 Jena, Germany

### ***Other Activities***

1. Group meeting presentation:
  - 19-01-2019
  - 28-03-2019
  - 25-05-2018
  - 05-10-2018
  - 19-01-2019
  - 10-05-2019
2. Perovskite Nanocrystals: the new generation of defect tolerant luminescent material. Speaker: Sameer Sapea



Università degli Studi di Genova  
Doctorate in  
Sciences and Technologies of  
Chemistry and Materials



Curriculum: Science and Technology of Materials

GIULIA SYLVA

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*

**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*

**Advisors:** Prof. Marina Putti (UNIGE), Dr. Valeria Braccini (CNR)

**Thesis Title:** Development of Iron-Based Superconducting wires and tapes for high field applications

**Thesis abstract**

The PhD project is a part of a collaboration activity between CERN and CNR-SPIN Genova (ADDENDUM FCC-GOV-CC-0086 to the Memorandum of Understanding for the FCC Study), which has the aim to develop superconducting materials alternative to Nb<sub>3</sub>Sn for high field applications within the FCC (Future Circular Collider) study. In the part of the project devoted to Iron-Based superconductors (IBS), the main objective is to study the possibility of developing a conductor in form of tape or wire in a scalable and cost-effective way.

In detail, the activity on IBS within this project has regarded:

- Development of Coated Conductors (CC) by deposition of films through Pulsed Laser Deposition (PLD) on metallic (Ni, Fe, or other suitable alloys) oriented templates prepared through a suitable alternation of cold deformation steps and annealing. In this framework we also collaborated with ENEA centre of Frascati that produces biaxially textured templates for YBCO which can be used also for IBS.
- Structural morphological and compositional characterization by means of X-ray diffraction analysis and SEM at SPIN and TEM, HRTEM and EPS at CERN.
- Transport critical current measurements in magnetic field.
- Preparation of powders of the BaFe<sub>2</sub>As<sub>2</sub> family for the development of Powder In tube (PIT) wires.

Moreover, to further study the possible application on Fe(Se,Te) at high magnetic field and in harsh environments, where strong radiation emissions are expected, such as in accelerators, proton irradiation of Fe(Se,Te) thin film was also studied. This activity was done in collaboration with Politecnico di Torino.

# ACTIVITY REPORT

## *Research Activity*

The research was mainly carried out at the Department of Physics of the University of Genova

### *Scientific Publications*

1. **G. Sylva**, E. Bellingeri, C. Ferdeghini, A. Martinelli, I. Pallecchi, L. Pellegrino, M. Putti, G. Ghigo, L. Gozzelino, D. Torsello, G. Grimaldi, A. Leo, A. Nigro and V. Braccini, 'Effects of high-energy proton irradiation on the superconducting properties of Fe(Se,Te) thin films' Superconductors Science and Technology 31 (2018) 054001 (10.1088/13616668/aab3bd)
2. **G. Sylva**, A. Malagoli, E. Bellingeri, M. Putti, C. Ferdeghini, A. Vannozzi, G. Celentano, S. C. Hopkins, A. Lunt, A. Ballarino, and V. Braccini, 'Analysis of Fe(Se,Te) Films Deposited On Unbuffered Invar 36' IEEE Transaction on Applied Superconductivity 29 (2019) 7300105 (10.1109/TASC.2019.2893585)
3. **G.Sylva**, A.Augieri, A.Mancini, A.Rufoloni, A.Vannozzi, G.Celentano, E.Bellingeri, C.Ferdeghini, M. Putti and V. Braccini, 'Fe(Se,Te) coated conductors deposited on simple RABiTS templates' Superconductors Science and Technology 32 (2019) 084006 (10.1088/1361-6668/ab0e98),
4. A. Leo, **G. Sylva**, V. Braccini, E. Bellingeri, A. Martinelli, I. Pallecchi, C. Ferdeghini, L. Pellegrino, M. Putti, G. Ghigo, L. Gozzelino, D. Torsello, S. Pace, A. Nigro, and G. Grimaldi 'Anisotropic Effect of Proton Irradiation on Pinning Properties of Fe(Se,Te) Thin Film' IEEE Transaction on Applied Superconductivity 29 (2019) 7300205 (10.1109/TASC.2019.2893592)
5. A. Abada et al-, 'FCC Physics Opportunities: Future Circular Collider Conceptual Design Report Volume 1' European Physics Journal C 79 (2019)474, (10.1140/epjc/s10052-019-6904-3)
6. Abada et al., 'FCC-ee: The Lepton Collider: Future Circular Collider Conceptual Design Report Volume 2' European Physical Journal Special Topics (2019)228 (10.1140/epjst/e2019-900045-4)
7. Abada et al., FCC-hh: The Hadron Collider: Future Circular Collider Conceptual Design Report Volume 3 European Physical Journal Special Topics (2019)228, (10.1140/epjst/e2019-900087-0)
8. Abada et al., HE-LHC: The High-Energy Large Hadron Collider Future Circular Collider Conceptual Design Report Volume 4, European Physical Journal Special Topics (2019) 228, (10.1140/epjst/e2019-900088-6)
9. N. Pompeo, A. Alimenti, K. Torokhtii, **G. Sylva**, V. Braccini, E. Silva, 'Microwave properties of Fe(Se,Te) thin films in a magnetic field: pinning and flux flow' Submitted on September 2019 to Journal of Physics: Conference Series (JPCS)
10. A. Leo, G. Grimaldi, A. Nigro, G. Ghigo, L. Gozzelino, D. Torsello, V. Braccini, **G. Sylva**, C. Ferdeghini, M. Putti, 'Critical current anisotropy in Fe(Se,Te) films irradiated by high-energy protons', submitted on September 2019 to Journal of Physics: Conference Series (JPCS)

### *Communications at Conferences*

#### *Oral communications:*

1. Effects of high energy proton irradiation on the superconducting properties of Fe(Se,Te) thin films (**G. Sylva**, E. Bellingeri, C. Ferdeghini, A. Martinelli, I. Pallecchi, L. Pellegrino, M. Putti, G. Ghigo, L. Gozzelino, D. Torsello, G. Grimaldi, A. Leo, A. Nigro, V. Braccini) at SuperFox 2018

### **Poster Communications:**

1. Effects of proton irradiation on the vortex dynamics of Fe(Se,Te) thin films- (**Giulia Sylva**, Valeria Braccini, Emilio Bellingeri, Alberto Martinelli, Marina Putti, Carlo Ferdeghini, Laura Gozzelino, Gianluca Ghigo, Antonio Leo, Gaia Grimaldi) at EUCAS 2017
2. Effects of proton irradiation on the superconducting properties of Fe(Se,Te) thin films (**Giulia Sylva**, Valeria Braccini, Emilio Bellingeri, Alberto Martinelli, Marina Putti, Carlo Ferdeghini, Laura Gozzelino, Gianluca Ghigo, Antonio Leo, Gaia Grimaldi) at ASC 2018
3. IBS wires and tapes produced with simple and scalable methods (**G. Sylva**, V. Braccini, A. Malagoli, E. Bellingeri, C. Ferdeghini, M. Putti, M. Lisitskiy, A. Provino, C. Bernini, A. Martinelli P. Manfrinetti, A. Augieri, G. Celentano, A. Mancini, A. Vannozzi, A. J. G. Lunt, Simon C. Hopkins, A. Ballarino) at FCC week 2019

### **Congresses Attended**

1. SuperFox 2018- Conference on superconductivity and functional oxides

## **Courseware**

### **Courses attended and passed (credits)**

### **Courses Given by Teachers of the Unige and IIT:**

1. Superconducting magnets for accelerators, Prof P. Fabbriatore (6 CFU)
2. Microscopic and Spectroscopic technique for the analysis of surface, Prof R. Buzio, A. Gerbi, L. Savio (3 CFU)
3. Functional ceramics- Prof. V. Buscaglia (3 CFU)
4. Electronic microscopy- Prof P. Riani (2 CFU)

### **Courses Given by invited experts (type A):**

1. Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials & Novel Materials for energy storage and conversion- T. Fassler at Chemistry department of University of Genova (2017)
2. An introduction to nanoscale magnetism for biomedical applications- N. Telling at IIT (2017)
3. Synthesis and characterization of magnetic nanomaterials for biomedical applications- D. at chemistry department of University of Genova (2018)
4. Basics of crystallography- M. Prato at IIT (2018)

### **National and International Schools or Workshops**

1. School on Science Management for Scientist and Engineers (SoSMSE 2017) at Physics department of University of Genova (6CFU)
2. Presence (Phd students as a bridge between Science and society)- DCCI Genova 27 October 2017
3. EASISchool on applied superconductivity at TU Wien – 3/7 September 2018 (2CFU)
4. Workshop on Microactuators (<http://www.vo2actuators.spin.cnr.it/workshop>)



### **Other Activities. Dissemination:**

1. 'Formazione alla ricerca scientifica' Tutor for Stage PLS 2017 at Physics department of University of Genova
2. 'Formazione alla ricerca scientifica' Tutor for stages PLS 2018 at Physics department of University of Genova
3. 'Formazione alla ricerca scientifica' Tutor for stages PLS 2019 at Physics department of University of Genova
4. ART & Science 2019 across Italy- preparation and disclosure of two seminars titled "Elettroni in Ballo" and an experimental activity on quantum levitation for high school students

### **Seminars attended:**

1. Metadevices and metasurfaces for the control of THz light – Dr. A. Andreone
2. Critical current density in NbTi and MgB<sub>2</sub> wires, FeSe and Ba(Fe<sub>0.92</sub>Co<sub>0.08</sub>)<sub>2</sub>As<sub>2</sub> bulks- Dr D. Gajda T. Cetner
3. TEM Cryogenic- Dr. Paolo Swuec
4. High pressure technology for wires manufacturing of MgB<sub>2</sub>, FeSeTe, another superconductor – Dr. Andrzej Morasky
5. Design of magnetic nano-architecture for biomedical applications- Dr. Davide Peddis
6. Thermoelectric materials- Dr Carlo Fanciulli
7. Superconductivity without doping in iron-based 1111 family: The ThFeAsN case- Dr. Toni Shiroka
8. MgB<sub>2</sub> thin films for SRF cavity applications - Dr. Xiaoxing Xi
9. The influence of high field pinning centres and layered structure on critical current density in MgB<sub>2</sub> wires- Dr. Daniel Gajda
10. Screening of mixed co-poly(ester carbonate) PEG-based nanoparticles for breast cancer therapy: an in vitro and biodistribution based approach- Dr. Robert Cavanagh
11. Using polymer 3D architecture, size and chemistry to control nanoparticle distribution for Duxorubicin drug delivery in vitro and in vivo-Dr Amanda Pearce
12. Organocatalyzed synthesis and characterization of a small library functionalisable co- poly(ester)-(carbonate)s initiated by varying pegylated architectures and labile- (metha)acrylate esters- Dr Vincenzo Taresco
13. Substrate preparation for Tl(1223) films - High temperature synthesis: Dr. Leveratto Alessandro
14. Advances in Tl(1223) deposition and characterization- Dr. Aisha Saba
15. YBCO tapes for beam screen- Dr. Sergio Calatroni
16. Analysis on new literature data on the surface impedance of superconductors in high magnetic fields- Dr. Ruggero Vaglio
17. Tl(1223) PIT Tapes- Dr. Leveratto Alessandro
18. Caloric effects in magnetic materials- Prof. Srikanth Hari
19. Engineering critical current density and n value in MgB<sub>2</sub> wires made with PIT technique- Dr. D. Gajda

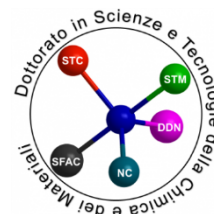
### **Others activities:**

1. Referee activity for scientific journals:
  - a. IEEE Transaction on Applied Superconductivity
  - b. European Physics Journal (EPJ)

2. The paper "Effects of high-energy proton irradiation on the superconducting properties of Fe(Se,Te) thin films" was selected as one of the CNR SPIN Highlights of 2018.
3. Attendance of the Course of Health and safety in the workspace at CNR SPIN, with final exam
4. Attendance of the course for the Utilization and the manipulation of pure technical and cryogenics gasses held by SOL in September 2019, with final exam
5. Member of the organization of the workshop IBS2App (Iron Based Superconductors: advanced towards Applications) that will be held in Santa Margherita in February 2020



Università degli Studi di Genova  
Doctorate in  
Sciences and Technologies of  
Chemistry and Materials



Curriculum: Chemical Sciences and Technologies

SILVIA VITA

**Start of the Doctorate Program:** *Novembre 1<sup>st</sup> 2016*  
**End of the Doctorate Program:** *October 31<sup>st</sup> 2019*  
**Advisors:** Prof. Silvia Vicini, Dr. Rico Ricotti

**Thesis Title:** New naval fillers for industrial applications (Yachting)

ACTIVITY REPORT

*Research activity*

The research activity was mainly carried out at Boero Bartolomeo SpA (Rivalta Scrivia, AL) and about two days per week at the DCCI, University of Genoa. From April 4 to July 4 2018 the research work was carried out at RISE (Research Institutes of Sweden) of Borås and Göteborg.

**Scientific Publications**

Original publications on ISI Journals:

1. M. Delucchi, E. Finocchio, M. Castellano, S. Vicini, **S. Vita**, G. Cerisola, R. Ricotti, Application of DSC and FTIR techniques for monitoring the curing process of epoxy fillers used for yacht application *Metallurgia Italiana*, 109 (2017) 107-110. Indexed on Scopus: 2-s2.0-85025174307. Indexed on WoS: 000437317200027. IF: 0.432.
2. S. Vicini, M. Castellano, M. Mauri, **S. Vita**, Alginate and alginate/hyaluronic acid membranes generated by electrospinning in wet conditions: relationship between solution viscosity and spinnability *Journal of Applied Polymer Science*, 135 (2018) 46390. Indexed on Scopus: 2-s2.0-85043389681. Indexed on WoS: 000428701200029. IF: 1.901.
3. M. Delucchi, E. Finocchio, M. Castellano, S. Vicini, **S. Vita**, G. Cerisola, R. Ricotti, A methodological approach for monitoring the curing process of fairing compounds based on epoxy resins *Progress in Organic Coatings*, 123 (2018) 20-26. Indexed on Scopus: 2-s2.0-85048888021. Indexed on WoS: 000444357000003. IF: 2.955.
4. **S. Vita**, R. Ricotti, C. Malegori, P. Oliveri, S. Vicini, M. Castellano, Univariate and multivariate strategies for the rheological tests evaluation: influence of additives in composite materials. *Journal of Applied Polymer Science* Submitted.

5. **Industrial development**, Epoyacht automatic mix (PATENTABLE); Product formulated during the first year of Ph.D. and commercially available from 2018.

### **Communications at Conferences**

#### **Oral Communications:**

1. **S. Vita**, Fillers for applications in the yachting, Macrogiovani, 22-23 June 2017, Trento.
2. **S. Vita**, R. Ricotti, S. Vicini, M. Castellano, Additivi reologici per Stucchi nautici, XVI Convegno Nazionale di Reologia, 18-21 June 2019, Roma

#### **Poster Communications:**

1. **S. Vita**, M. Mauri, R. Ricotti, M. Castellano, S. Vicini, The additives for naval filler (yachting), Abstract Booklet of EUPOC 2017, Polymer and Additive Manufacturing: from Fundamentals to Applications, 21-25 May 2017, Gargnano (BS), p.63.
2. **S. Vita**, R. Ricotti, M. Legrottaglie, E. Pinori, M. Castellano, S. Vicini, Influence of wetting agent on rheological properties of composite materials for naval applications, 23-26 April 2019, Palermo.

#### **Congresses Attended**

1. EUPOC 2017: Polymer and Additive Manufacturing: from Fundamentals to Applications, 21-25 May 2017, Gargnano (BS).
2. Macrogiovani, 22-23 June 2017, Trento.
3. European Coating Show, 18-21 March 2019, Nuremberg.
4. Eurofillers Polymerblends, 23-26 April 2019, Palermo. (Grant for merit).
5. XVI Convegno Nazionale di Reologia, 18-21 June 2019, Roma.

## **Courseware**

#### **Courses attended and passed**

1. Analisi Multivariata di dati chimici, Proff. Leardi, Oliveri, Casali. (3 CFU)
2. Soft Matter, Prof.ssa Relini. (2 CFU)
3. Industrial Catalysts and Adsorbents, Prof. Busca. (2 CFU)
4. Synthesis, structure and functional properties of intermetallic compounds, Prof.ssa Saccone. (2 CFU)
5. Basic Scanning and Transmission Electron Microscopies, Prof.ssa Riani. (3 CFU)

#### **Courses given by invited experts:**

1. Prof. T. Fässler: part 1 "Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials"; part 2 "Novel Materials for energy storage and conversion" – 11 May 2017.
2. Prof. A. Passerone: "Superfici ed interfacce in sistemi metallo-ceramici" – 16 and 19 May 2017.
3. Prof. J. Sereni "Cryocooler materials for Adiabatic Demagnetization: Comparison between paramagnetic salts and intermetallic compounds" – 4 July 2017.
4. Prof. P. Rogl "Advanced Thermoelectric Materials for Renewable Energy" – 11 and 13 June 2019

#### **National and International Schools or Workshops**

1. Scuola di Reologia Industriale – 3-7 September 2017, Valeggio sul Mincio (VR). (Grant for merit).

2. Scuola di Experimental Design – 25-29 September 2017, Genova.
3. Scuola di Analisi Multivariata – 29 January - 2 February 2018, Genova.
4. Combining NIR spectroscopy and Chemometrics – 14-18 January 2019, Milano.
5. Workshop “Trends in wood coatings” – 13 December 2018, Torino.
6. Workshop “Anton Paar – Dynamic Mechanical Analysis” – 12 March 2019, Rivoli (TO).
7. Workshop “Mettler-Toledo – Caratterizzazione dei Materiali” – 2 October 2019, Modena.

### ***Seminars Attended***

1. Dr. F. Locardi: “Analisi termica accoppiata alla gas cromatografia e spettrometria di massa. Un potente strumento per la caratterizzazione dei materiali” – 13 June 2017.
2. Proff. M. Grotti e P. Rivaro, “Il Contributo Del DCCI al Programma Nazionale Di Ricerche In Antartide” – 27 February 2018.
- 3-6 Dr. H. Witthoff, Siltech AB – Thermoset education certificate (16 hours equivalent to 4 seminars).
7. Ing. R. Ricotti, Sig. P. Stortoni, “Prodotti per il settore Yacht e loro caratteristiche” – 25 September 2018, Rivalta Scrivia (AL).
8. Prof. J. Sereni “New perspectives for low temperature refrigeration with advanced magneto-caloric materials” – 13 November 2018.
9. Dr. F. Cagliaris “Anomalous transport properties in Weyl semimetals” – 19 November 2018.
10. Ing. S. Garofoli, Sig. P. Stortoni, “Nuovi sviluppi nel settore Antifouling” – 6 December 2018, Rivalta Scrivia (AL).
11. Dr. P. Tanasini, “Process development: the role of thermal safety investigations” – 7 January 2019.
12. Prof. P. Melchiorre, “Organic synthesis in the excited state: enhancing the potential of organocatalysis with light” – 25 January 2019.
13. Dr. S. Cahen “Searching for superconductivity in graphite intercalated with hydrogen-based compounds” – 4 February 2019.
14. Dr. E. Aghemo, L. Fusani, “Additivi per materiali polimerici” – 24 May 2019.
15. Various speakers “An introduction to metal nanoparticles and nanoalloys” – 4 June 2019.
16. Ing. R. Ricotti, Sig. P. Stortoni “Nuovi sviluppi nella formulazione del colore: pigmenti metallizzati e perlescenti ad uso nautico” – 10 June 2019, Rivalta Scrivia (AL)
17. Prof. C. Santoro, “Insights in platinum group metal (PGM-free) catalysts for oxygen reduction reaction” – 5 September 2019.
18. Dr. S. Uwe “Science of Synthesis” – 9 October 2019

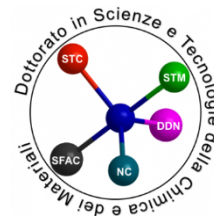
### ***Other Activities***

1. Attività di supporto alla didattica II anno: 8 ore per Chimica fisica 1 con laboratorio (LT in CTC) e 16 ore per Laboratorio di chimica industriale (LM in CI).
2. Attività di supporto alla didattica III anno: 28 ore per Chimica fisica 1 con laboratorio (LT in CTC) e 8 ore per Laboratorio di chimica industriale (LM in CI).
3. Collaborazione coordinata continuativa con Università degli Studi di Genova (DCCI) – Supporto alla gestione di Stage rivolti agli istituti di istruzione secondaria di secondo grado nell’ambito del Piano Nazionale Lauree Scientifiche (PNLS) e Alternanza Scuola-Lavoro (ASL) Area Chimica – 25-29 marzo 2019.
4. Scientific explainer, Festival della Scienza 2016 Laboratory “Plastica: uso e riuso”).
5. Scientific explainer, Festival della Scienza 2017 (Laboratory “Alimenti a Contatto”).
6. Scientific explainer, Festival della Scienza 2018 (Exhibit “Starlight: le stelle in una stanza”).
7. Scientific explainer, Festival della Scienza 2019 (Laboratory “Attraverso lo specchio”).
8. Scientific explainer, Moleday 2017.

9. Scientific explainer, Moleday 2018.
10. Scientific explainer, Moleday 2019.



Università degli Studi di Genova  
Doctorate in  
Sciences and Technologies of  
Chemistry and Materials



Curriculum: Chemical Sciences and Technologies

GABRIELLA VITALI FORCONESI

Start of the Doctorate Program: November 1<sup>st</sup>, 2016

End of the Doctorate Program: October 31<sup>st</sup>, 2019

Advisor: Prof. Renata Riva

**Thesis Title:** Development of novel bio-based building blocks and their application in organic synthesis and materials science

## ACTIVITY REPORT

### *Research Activity*

A research period of 6 months (January 27<sup>th</sup> - July 27<sup>th</sup> 2019) was spent at the University of Stellenbosch (South Africa) under the Supervision of Prof. Bert Klumperman and Dr. Rueben Pfukwa, within the Project “Synthesis, Characterization, Structure and Properties of Novel Biodegradable Polyesters (BIODEST)” that is funded under the Research and Innovation Staff Exchange (RISE) Scheme (H2020-MSCA-RISE-2017-778092).

### *Scientific Publications*

1. **Gabriella Vitali Forconesi**, Luca Banfi, Andrea Basso, Chiara Lambruschini, Lisa Moni, and Renata Riva, “Synthesis of polyoxygenated heterocycles by diastereoselective functionalizations of a bio-based chiral aldehyde exploiting the Passerini reaction”, *Molecules*, 2019, submitted.
2. **Gabriella Vitali Forconesi**, Lisa Moni, Renata Riva et al. “Chemoenzymatic Total Synthesis of 4-epi-Bengamide E: a fruitful example of combination of renewable sources, Multicomponent Reaction, and Biocatalysis” manuscript under preparation.

## **Communications at Conferences**

### **Oral Communications:**

1. **G. Vitali Forconesi**, L. Moni, R. Riva, "Biocatalysis and MCRs: a useful combination for the synthesis of bio-based polyfunctionalized heterocycles", EAMHC-2019 10th Eurasian Meeting on Heterocyclic Chemistry, Milano Marittima-Cervia (Italy), 15th - 19th September 2019.

### **Poster Communications:**

1. **G. Vitali Forconesi**, L. Moni, R. Riva "Application of MCRs to the stereoselective synthesis of heterocycles scaffolds starting from chemoenzymatically obtained chiral aldehydes" GIFC-2018- Giornate Italo-Francesi della chimica, Genova (Italy), 16th – 18th April 2018.
2. **G. Vitali Forconesi**, L. Moni, R. Riva, "Stereoselective multicomponent reactions of biobased chiral aldehydes derived from chemoenzymatic strategies", ISOS 2017-XLII International Summer School on Organic Synthesis "A. Corbella", Gargnano (Italy), 18th - 22nd June 2017.
3. **G. Vitali Forconesi**, L. Moni, R. Riva, "Biocatalysis and MCRs: a potential green strategy for the synthesis of high added-value compounds starting from biomass", ISOC 2017-11th International School of Organometallic Chemistry, San Benedetto del Tronto (Italy), 2nd – 6th September 2017.

### **Congresses Attended**

1. IX Giornate Italo- Francesi di Chimica, Genova (Italy), 16-18 April 2018.
2. 13<sup>th</sup> International Conference on Advanced Polymers via Macromolecular Engineering (APME 2019), Stellenbosch (South Africa), 15-18 April 2019.
3. 10<sup>th</sup> Eurasian Meeting on Heterocyclic Chemistry (EAMHC-2019), Milano Marittima-Cervia (Italy), 15<sup>th</sup> - 19<sup>th</sup> September 2019

### **National and International Schools or Workshops:**

1. 5<sup>th</sup> Workshop "Programma PhD: La formazione post lauream e il mondo del lavoro - Nell'Industria Chimica, 24 Mai 2017, Polytechnic School, University of Genova.
2. Multiphoton at the Cutting Edge: Sales Specialist Confocal Microscopy, Leica Microsystems (Workshop), 11 October 2017, Genoa, Italy.
3. POLYMAT DAY, 01 December 2017, Auditorium Carlos Santamaria – University of the Basque country, San Sebastian, Spain.
4. Workshop on Polymer Crystallization. (03 – 05 September 2018, Genoa, Italy)

## **Courseware**

### **Courses Given by Teachers of the University of Genova (B-type courses):**

1. Organic photochemistry- Prof. Basso (2 CFU)
2. Diversity Oriented Synthesis of Heterocyclic Compounds- Prof. Riva and Dr. Moni (2 CFU)
3. Metodologia della ricerca sperimentale - Experimental Design - Prof. Grotti and Prof. Leardi (3 CFU)
4. Multivariate analysis of chemical data - Prof. Leardi, Prof. Olivieri and Prof. Casali (3 CFU)
5. Perspectives on bioinorganic chemistry - Prof. De Negri (2 CFU)



### **A-type Courses:**

1. Superhard materials: Structural chemistry of boron and borides, Prof. Peter Rogl, University of Vienna, 6 - 7 June 2017, DCCI.
2. Publishing papers and strategies to visualize the scientific productivity, Prof. José Manuel Domínguez González, University of Vigo (Spain), 27 June 2017, DICCA, University of Genoa
3. Recent advances in computer-aided drug design, prof. Tiziano Tuccinardi, 16 October 2017, DIFAR, University of Genoa

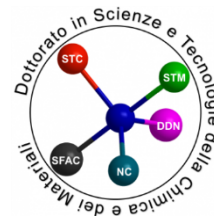
### **Seminars Attended:**

1. Vincenzo Buscaglia from ICMATE-CNR, "Synthesis of high permittivity nanoparticles by hydrothermal and solvothermal methods" (29th March 2017, CNR – Genoa).
2. Paola Stagnaro, ISMAC-CNR, "Polymer-based Composites: Process-Structure Properties Relationship" (29th March 2017 in CNR – Genoa).
3. Leontin Padurariu, "Al I. Cuza" University, Romania, "3D Finite Element Method modelling of dielectric and ferroelectric properties of composite systems" (29th March 2017, CNR – Genoa).
4. Lavinia Curecheriu, "Al I. Cuza" University, Romania, "Electrical properties of chitosan-based composites: Towards active dielectrics for flexible electronics" (29th March 2017, CNR – Genoa).
5. Davide Comoretto, DCCI - UNIGE, "All-Polymer Nano-Photonics: from Lasers to Sensors" (29th March 2017, CNR – Genoa).
6. L. Zerroual, UFAS-1, towards a new technology of lead acid batteries (10th May 2017) in University of Setif -1, Algeria).
7. T. Aissaoui, UFAS-1, Essential steps for Algerian researcher to target ISI journals (10th Mai 2017 in University of Setif -1, Algeria).
8. Richard E. Palmer, University of Birmingham, "Atomic structure and mass-production of size-selected nanoparticles (clusters)" (30th Mai 2017, DIFI – Genoa).
9. S. Riva, CNR – Milano, "Un caso di proficua collaborazione: biocatalisi e prodotti naturali" (16th June 2017, DCCI – Genoa).
10. Jason K. Sello, Brown University of Providence (USA), "Novel small molecules, targets, and strategies in anti-infective development" (3th July 2017, DCCI – Genoa).
11. Julian Sereni, Instituto Balseiro Centro Atomico Bariloche (Argentina), "Cryocooler materials for Adiabatic Demagnetization: Comparison between paramagnetic salts and intermetallic compounds" (4th July 2017, DCCI – Genoa).
12. Paolo Mele, Muroran Institute of Technology, Hokkaido (Japan), "On research activities at Muroran Institute of Technology" (24th July 2017, DCCI – Genoa).
13. Nevena Marinova, University of the Basque country (Spain), "Light and oxygen resistant methyl ammonium lead iodide perovskite stabilized with hindered amine light stabilizer" (23rd Febrary 2018, Auditorium Korta – San Sebastian, Spain).
14. Nadia Lotti, University of the Bologna (Italy), "New biobased polyesters: structure-property relationship" (09th March 2018, Physics Department – San Sebastian, Spain).
15. Ulrich S. Schubert, Friedrich-Schiller-University Jena (Germany), "Polymers for batteries" (11th Mai 2018, Auditorium Korta – San Sebastian, Spain).

16. Thomas Thurn-Albrecht, University of Halle-Wittenberg (Germany), "Microscopic Observation of Interface-Induced Crystallization via Prefreezing in Polymers Melts" (16th June 2018, Auditorium Korta – San Sebastian, Spain).



Università degli Studi di Genova  
Doctorate in  
Sciences and Technologies of  
Chemistry and Materials



Curriculum: Chemical Sciences and Technologies

**BAO WANG**

**Start of the Doctorate Program:** *November 1<sup>st</sup>, 2016*

**End of the Doctorate Program:** *October 31<sup>st</sup>, 2019*

**Advisor:** Prof. Dario Cavallo

**Thesis Title:** Nucleation of semi-crystalline polymers

## ACTIVITY REPORT

### *Research Period Abroad*

8-months Internship at Eindhoven University of Technology, Netherlands, funded by the Erasmus+ internship project.

Period: 15 January 2019 - 15 September 2019

### *Scientific Publications*

1. **Wang B**, Menyhard A, Alfonso G C, et al. Differential scanning calorimetry study of cross-nucleation between polymorphs in isotactic poly(1-butene). *Polymer International*, 2019, 68(2): 257-262. DOI: 10.1002/pi.5595
2. **Wang B**, Wen T, Zhang X, et al. Nucleation of Poly (lactide) on the Surface of Different Fibers. *Macromolecules*, 2019, 52(16): 6274-6284. DOI: 10.1021/acs.macromol.9b01078
3. **Wang B**, Dario Cavallo, Bin Zhang, Jingbo Chen, Evolution of chain entanglement under large amplitude oscillatory shear flow in isotactic polypropylene. *Polymer*, 2019. DOI: 10.1016/j.polymer.2019.121899

## ***Communications at Conferences***

### ***Poster Communications:***

1. **Bao Wang**, Dario Cavallo, Bin Zhang, Jingbo Chen. "Evolution of chain entanglement under large amplitude oscillatory shear flow in isotactic polypropylene" 9th International Symposium on Engineering Plastics « EP2019». (07-10 August 2019, Yinchuan, China)

### ***Congresses Attended***

1. 9<sup>th</sup> International Symposium on Engineering Plastics « EP2019». (07-10 August 2019, Yinchuan, China).

## ***Courseware***

### ***Type B courses:***

1. "Surface Science", Prof. Luca Vattuone;
2. "Basic Scanning and Transmission Electron Microscopies", Prof. Paola Riani.

### ***Seminars***

3. "Anomalous transport properties in Weyl semimetals" Federico Cagliaris, from Leibniz Institute for Solid State and Materials Research (IFW), Dresden, Germany. (19 November 2018 DIFI, Genova).
4. "New perspectives for low temperature refrigeration with advanced magneto-caloric materials" Julian G. SERENI (Low Temperature Division - Centro Atomico Bariloche - San Carlos de Bariloche - Argentina). (13 November 2018 DCCI, Genova).
5. "Materiali organici nanostrutturati a base di Carbonio, Azoto e Boro" Dott. Paolo Giusto (Max Planck Institute of Colloids and Interfaces, Department of Colloid Chemistry, Potsdam - Golm, Germany. (29 November 2018 DCCI, Genova).
6. "Process development: the role of thermal safety investigations" Pietro Tanasini (PhD, Process Development Manager di Huntsman Advanced Materials, Sàrl-Monthey, CH). (07 January, 2019 DCCI, Genova).
7. "Insights in platinum group metal (PGM-free) catalysts for oxygen reduction reaction" Carlo Santoro, Associate Professor from Department of Engineering, Design and Mathematics University of the West of England, Bristol. (September 5, 2019 DCCI, Genova).