

UNIVERSITY OF GENOVA

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

XXX 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 XXX cycle, 11 out of 25 students were foreigner (44%).

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 12 members, and by a Director.

For the XXX cycle the board of professors was formed by:

- Tiziano Bandiera IIT
- Antonio Barbucci DICCA
- Raffaella Boggia DIFAR
- Olga Bruno DIFAR
- Gabriele Cacciamani DCCI
- Fabio Canepa DCCI
- Maurizio Canepa DIFI
- Gabriele Caviglioli DIFAR
- Massimo Colombo IIT
- Antonio Comite DCCI
- Davide Comoretto DCCI
- Carlo Ferdeghini CNR
- Maurizio Ferretti DCCI
- Paola Fossa DIFAR
- Gianpiero Garau IIT
- Federica Gastaldo DCCI
- Maria Carmela Ianni DCCI
- Roman Krahne IIT
- Silvia Lanteri DIFAR
- Riccardo Leardi DIFAR
- Emanuele Magi DCCI
- Liberato Manna IIT
- Iwan Moreels IIT
- Teresa Pellegrino IIT
- Giovanni Petrillo DCCI
- Mirko Prato IIT
- Marina Putti DIFI
- Gianguido Ramis DICCA
- Annalisa Relini DIFI
- Renata Riva DCCI
- Adriana Saccone DCCI
- Silvia Schenone DIFAR
- Carla Villa 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 Pharmaceutical Sciences (DISCIFAR), Dep. of Chemistry and Pharmaceutical and Food Technologies (DICTFA), Department of Chemical and Process Engineering "G.B. Bonino" (DICheP), 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 School in
Sciences and Technologies of
Chemistry and Materials**

Curriculum: Nanochemistry

Guilherme Almeida

Start of the Doctorate Program *November 1st, 2014*

End of the Doctorate Program *November 1st, 2017*

Advisors

Dr. Liberato Manna

Prof. Davide Comoretto

Thesis Title

Colloidal synthesis and characterization of non-conventional semiconductor nanomaterials

Thesis abstract

Herein is reported an investigation of the colloidal synthesis and characterization of novel nanomaterials with semiconducting properties. These include single-layer In_2Se_3 nanosheets, antiferromagnetic CuFeS_2 nanopyramids and luminescent CsPbBr_3 nanocubes. Original synthetic protocols were devised and the nanomaterials were characterized with a variety of chemical, structural, optical and electrical techniques. Furthermore, these results are preceded by a review of the state-of-the-art for each material class, their relevance to the field is highlighted and further work is proposed.

ACTIVITY REPORT

Research Activity

The research activity was mainly carried out at the IIT
Please indicate here if you have spent research periods in foreign countries.

Scientific Publications

Original publications on ISI Journals:

1. Ghosh et al., Colloidal CuFeS₂ nanocrystals: intermediate Fe d-band leads to high photothermal conversion efficiency, Chem. Mat., 2016, 28, pp 4848-4858
2. Almeida et al., Colloidal Monolayer β -In₂Se₃ Nanosheets with High Photoresponsivity, J. Am. Chem. Soc., 2017, 139, pp 3005–3011
3. Almeida et al., Changing the Dimensionality of Cesium Lead Bromide Nanocrystals by Reversible Postsynthesis Transformations with Amines, Chem. Mater., 2017, 29, pp 4167–4171
4. Almeida et al., The role of acid base chemistry in the synthesis of CsPbBr₃ nanocrystals, manuscript under submission

Communications at Conferences

Poster Communications:

1. Colloidal synthesis and optoelectronic properties of In₂Se₃ nanosheets (presented at ISN2A, ESONN summer school and Graphene 2017)

Oral Communications:

1. Colloidal synthesis and optoelectronic properties of In₂Se₃ nanosheets (Nanoge September meeting 2017, Barcelona). A second oral presentation regarding the In₂Se₃ work will be given at MRS Boston in November 2017.

Congresses Attended

1. Second international symposium on nanoparticles/nanomaterials and applications (ISN2A)
18th-21st January 2016
2. Graphene 2017, Barcelona
28th-31st March 2017
3. Nanoge September meeting, Barcelona
4th – 8th September 2017

Courseware

Courses attended and passed

1. Nanocomposites: processing and characterization by Dr. L. De Trizio and Dr. M. Arciniegas (1 credit)
Taught by: Dr. L. De Trizio, Dr. M. Arciniegas
Credits: 1
2. X-ray based techniques: XRD, XPS and XAS by Dr. M. Prato (1 credit)
Taught by: Dr. M. Prato
Credits: 1
3. Insights on electron microscopy by Dr. R. Brescia and Dr. A. Genovese (1 credit)
Taught by: Dr. R. Brescia, Dr. A. Genovese
Credits: 1
4. Opto-electronic properties of semiconductor quantum dots
Taught by: Dr. I. Moreels
Credits: 1
5. Energy storage and catalysis
Taught by: Dr. M. Colombo and Dr. S. Monaco
Credits: 1
6. Basics of crystallography
Taught by: Dr. L. Manna
Credits: 1
7. Optical properties of materials
Taught by: Prof. M. Canepa and Dr. F. Bisio
Credits: 3
8. Electrical and Raman characterization techniques
Taught by: Roman Krahne
Credit: 1
9. Science and technology of two-dimensional crystals
Taught by: F. Bonaccorso
Credits: 1
10. NIR spectroscopy: theory and applications
Taught by: T. Cattaneo and R. Giangiacomo
Credits: 1
11. Conventional and unconventional superconductivity: an overview
Taught by: E. Bauer
Credits: 1
12. Electronic properties of solids
Taught by: L. Manna
Credits: 3 credits
13. Laser-matter interaction
Taught by: Marti Duocastella
Credits: 4 credits

National and International Schools or Workshops (program)

1. Corso nazionale di introduzione alla fotochimica (06-10/06/2016, Bologna, Italy)
2. European school on nanosciences and nanotechnologies (28/08-17/09/2016, Grenoble, France)
3. Compass meeting (25th-26th September 2017, Camogli)
Meeting with several international research groups working in the field of nanocrystals

Seminars Given

1. Colloidal synthesis of In_2Se_3 nanosheets – group meeting 10th December 2016
2. Perovskite meeting (18th-19th May 2017, Milano)
Progress meeting with several Italian research groups working in the field of lead halide perovskites.

Seminars Attended

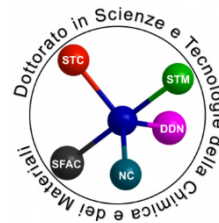
1. *Semiconductor nanocrystals laser structures*
Speaker: Dr. F. Di Stasio
2. *Plasmonic nanomaterials*
Speaker: Dr. H. Mehdi
3. *Designing organometallics for material science: application for solar cells and scintillators*
Speaker: Dr. G. Bertrand
4. *Colloidal quantum dot optoelectronics: photodetectors and solar cells*
Speaker: Prof. G. Konstantatos
5. *Using colloidal quantum dots to boost photovoltaic cell performance*
Speaker: Dr. M. Kazes
6. *Versatile fabrication of highly porous cryogels from noble metal nanoparticles*
Speaker: Axel Freytag
7. *Yb and Eu s correlated electron systems*
Speaker: Dr. Iwan Curlik
8. Semiconductor nanocrystals: discovery, milestones and recent theoretical developments
Speaker: A.L. Efros,
Date: 20/10/2016
9. Spatio-temporal visualization of atomic motions in low-dimensional materials
Speaker: G. M. Vanacore
Date: 03/05/2016
10. First-principles predictions of substrate effects on silicone
Speaker: U. Schwingenschloegl
Date: 09/05/2016
11. Perovskites: an old material for the third generation of PV solar panels
Speaker: L. Miranda Perez
Date: 21/04/2016

12. Colloidal nanoparticles and applications
Speaker: A.G. Kanaras
Date: 28/04/2016
13. Hydration induced spin glass state in a frustrated Na-Mn-O triangular lattice
Speaker: I. Bakaimi
Date: 28/05/2016
14. Visualizing and controlling optoelectronic processes in lead halide perovskites
Speaker: Alexander Weber-Bargioni,
Date: 14th November 2016
15. From chemical complexity to functional complexity: tailoring multifunctional low dimensional materials and devices
Speaker: Paolo Samorì
Date: 14th November 2016
16. van der Waals Assembly of 2D Materials for Device Applications
speaker: Gwan-Hyoung Lee
date: 16th January 2017
17. Photoactive systems for solar energy conversion, luminescence and catalysis
Speaker: Nicola Armaroli
Date: 27th January 2017
18. Showcasing catalysis research at Toyota Central R&D Labs.
Speaker: Takahiro Ikeda
Date: 1st February 2017
19. Interplay of electronic and dynamical processes in organohalide perovskites
Speaker: Dr. Filippo De Angelis
Date: 14th March 2017
20. Showcasing current research activities in D. Talapin's group
Speaker: Dmitri Talapin
Date: 26th May 2017
21. Showcasing current research activities in F. Toma's group
Speaker: Francesca Maria Toma
Date: 14th June 2017



Università degli Studi di Genova

Doctorate in Sciences and Technologies of Chemistry and Materials



Curriculum: Sciences and Technologies of Materials

GREGORIO BOCCALERO

Start of the Doctorate Program *November 1st, 2014*
End of the Doctorate Program *October 31st, 2017*
Advisors *Prof. Corrado Boragno (DIFI)*
Thesis Title *DEVELOPMENT OF A NOVEL COUPLED-MODE FLUTTERING ENERGY HARVESTER
THROUGH ELECTROMAGNETIC COUPLING AND DIELECTRIC ELASTOMER GENERATORS*
Thesis abstract

The topic of the research is the development of a novel energy harvester exploiting fluids in motion. FLEHAP device (Fluttering Energy Harvester for Autonomous Powering, patent pending), conceived and developed at DIFI of University of Genova, is an aero-elastic flutter-based system of an airfoil exploiting an electromagnetic coupling (EMc) and smart materials to extract electrical energy from the wind. It is performed the experimental study of the aeroelastic system through different prototypes, highlighting the main operating parameters and their correlations, analyzing the kinematics and the fluid dynamics aspects. The design of Dielectric Elastomer Generator materials (DEGs), their realization, characterization and application in the FLEHAP device are carried out. Electrical conversion and storage solutions are investigated for both the EMc and DEGs. The topics discussed are developed in terms of Research and direct technological application.

ACTIVITY REPORT

Research Activity

Research Period Abroad

The Abroad Period Research has been developed in the Laboratoire de Mécanique des Contacts et des Structures (LAMCOS) and in the laboratories of Ingénierie des Matériaux Polymères (IMP) of the Institut National des Sciences Appliquées (INSA) of Lyon, France, and partially in the Laboratoire de génie électrique de Grenoble (G2Elab) of the Institut Polytechnique de Grenoble (INP), France, from June to September 2016.

Scientific Publications

Published:

- 1) "A new energy harvester for fluids in motion", C. Boragno, G. Boccacero, Proc. SPIE 9431, Active and Passive Smart Structures and Integrated Systems 2015, 94310G; doi: 10.1117/12.2084591, April 2015
- 2) "FLEHAP: A Wind Powered Supply for autonomous Sensor Nodes", G. Boccacero, C. Boragno, D.D. Caviglia, R. Morasso, J. Sens. Actuator Netw. 5(4), 15; doi:10.3390/jsan5040015, October 2016

- 3) "Fluttering conditions of an energy harvester for autonomous powering", S. Olivieri, G. Boccalero, A. Mazzino, and C. Boragno, *Renew. Energy*, vol. 105, pp. 530–538, doi.org/10.1016/j.renene.2016.12.067, December 2016
- 4) "Power harvesting by electromagnetic coupling from wind-induced limit cycle oscillations" G. Boccalero, C. Boragno, S. Olivieri, A. Mazzino, *Smart Materials and Structures*, 26, 095031, August 2017
- 5) "A Sensor Node Driven by Air Flow", G. Boccalero, C. Boragno, R. Morasso, D.D. Caviglia, *IEEE NGCAS 2017*, DOI: 10.1109/NGCAS.2017.26, September 2017
- 6) "Fluttering Energy Harvester for Autonomous Powering (FLEHAP): a synergy between EMc and Dielectric Elastomers Generators", G. Boccalero, C. Boragno, S. Olivieri and A. Mazzino, *Procedia Engineering*, 199 3428–3433, 2017
- 7) "Fluttering Energy Harvester for Autonomous Powering (FLEHAP): aeroelastic characterization and preliminary performance evaluation", S. Olivieri, G. Boccalero, C. Boragno and Andrea Mazzino, *Procedia Engineering*, 199 3474-3479, 2017

On writing:

- 8) "Aero-dynamic repercussions on a novel fluttering Energy Harvester", C. Boragno, G. Boccalero, *Journal of Fluids and Structures*, on re-writing
- 9) "Soft, hyper-elastic and highly-stable organo-clay silicone dielectric elastomer for Energy Harvesting applications", G. Boccalero, C. Jean-Mistral, M. Castellano, *Royal Society of Chemistry*, on writing

Communications at Conferences

Oral communications:

- 1) "FLEHAP: Fluttering Energy Harvester for Autonomous Powering" in the Workshop "Dynamics of Nonlinear Materials and Structures in Energy Harvesting" on 13th February 2015 in Lublin (Poland)
- 2) "Energy Harvesting from fluids in motion by means of DEGs and EMc in a coupled-mode fluttering system" in "Journées Nationales sur la Récupération et le Stockage d'Énergie" (JNRSE2017), on May 9th-10th 2017 in Lyon (France).
- 3) "A Sensor Node Driven by Air Flow", in *New Generation of Circuits and System (NGCAS2017)* on 26th September 2017 in Genova (Italy)
- 4) "Fluttering Energy Harvester for Autonomous Powering (FLEHAP): a synergy between EMc and Dielectric Elastomers Generators" in the X International Conference on Structural Dynamics (EURODYN 2017) on 11th September 2017 in Rome (Italy)

Poster Communications:

- 1) "FLEHAP: Fluttering Energy Harvester for Autonomous Powering", in "Devices, Materials and Structures for Energy Harvesting", on 17th February 2016 in Brno (Czech Republic)
- 2) "Novelties and perspectives of a low wind speed Fluttering Energy Harvester for Autonomous Powering (FLEHAP)", in "Devices, Materials and Structures for Energy Harvesting and Storage", on 18 May 2017 in Oulu (Finland)
- 3) "Self-powering from fluids in motion by a coupled-mode fluttering device", electronic poster with presentation, in "Smart System Integration and Energy Harvesting" on 26-28 June 2017, La Valletta (Malta)

Congresses Attended

- 1) 1st International Conference on Dielectrics (ICD 2016), 3-7 July 2016, Montpellier, France
- 2) X International Conference on Structural Dynamics, (EURODYN 2017), 10-13 September, Rome.

Courseware

Courses attended and passed (10)

Courses Given by Teachers of the Unige and IIT:

- 1) Functional magnetic materials, Prof. F. Canepa, DCCI, Unige (2)
- 2) Elementary Electronic Structure of Solids, Prof. L. Manna, IIT (3)
- 3) Aerodynamics, Prof. A. Bottaro, DICCA, Unige (3)

- 4) Polymeric Nanocomposites, O. Monticelli, DCCI, Unige (2)

Courses Given by invited experts:

- 1) "Yb and Eu Strongly Correlated Electron Systems: from Experiment to Interpretation of Physical Properties", 21st-22nd April 2015, Dr. Ivan Curlik, University of Presov, Slovacchia
- 2) "Green Analytical Chemistry", 26th-27th May 2015, Prof. Estrella Espada Bellido, University of Cadiz, Spain
- 3) "Modern Materials for Energy Saving (Renewable Energy)", 9th-10th June 2015, Prof. Peter Rogl, University of Wien, Austria
- 4) "Low and Very Low Temperatures: Methods of Producing and Measuring Cryogenic Temperatures", 17-18 February 2016, Dr. Ivan Curlik, University of Presov, Slovacchia
- 5) "Physic in Extreme conditions", 5-6 April 2016, Prof. M Reiffers, DrSc., FInstP, Presov University, Slovakia

National and International Schools or Workshops

- 1) "Dynamics of Nonlinear Materials and Structures in Energy Harvesting" 12-13 February 2015, Lublin (Poland)
- 2) "Devices, Materials and Structures for Energy Harvesting", 16-17-February 2016, Brno (Czech Republic)
- 3) "Devices, Materials and Structures for Energy Harvesting and Storage", 17-18 May 2017, Oulu (Finland)
- 4) "Smart System Integration and Energy Harvesting", 26-28 June 17, La Valletta (Malta)

Seminars

Attended

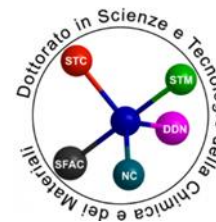
- 1) "Photochemically generated phenyl cations as tunable and versatile intermediates", 13rd January 2015, Dott. Stefano Protti, University of Pavia
- 2) "Polymers and Composites from Renewable Resources", 24th September 2015, Prof. A. Gandini, Institut Polytechnique de Grenoble (Grenoble INP), FR
- 3) "Interface behavior between different types of dielectrics", 3rd July 2016, Prof. Gérard Touchard, Univ. of Poitiers (France), in Montpellier, France
- 4) " α and β nucleation in the crystallization of isotactic Polypropylene", 11th October 2016, Stan Looijman, Eindhoven (Holland)
- 5) "Novel small molecules, targets and strategies in anti-infective development", 3rd July 2017, Prof. Jason K. Sello, Brown University of Providence (USA)
- 6) "Cryocooler materials for Adiabatic Demagnetization: Comparison between paramagnetic salts and intermetallic compounds", 4th July 2017, Prof. Julian Sereni, Balseiro Centro Atomico Bariloche (Argentina)

Given

- 1) "Energy Harvesting through Electromagnetic coupling and Dielectric elastomer generators" on 11th July 2016 in INSA de Lyon (France)

Other Activities

- 1) Participation to Italian physics and engineering graduation thesis competition on new technologies for sustainable development "Technology for human beings", promoted by Prysmian Group & Human Foundation, on 10th February 2015, in where it won the 3rd place
- 2) Participate to "SMARcup Liguria 2015", winning the 1st place of "Smart and Clean" category (4th in Italy)
- 3) Participate to Start Cup of University of Genova, winning the 1st place, 11th November 2015
- 4) EHLAB, a University spin-off has been constituted on December 2016, with the aim of applying the FLEHAP device in different Internet of Things scenarios (smart agriculture, environment monitoring, structural monitoring ...)
- 5) Laboratory lessons on basic concepts of fluid-solid-interactions and energy harvesting, imparted to engineering master degree student of DICCA on 17th March 2016 and 22nd March 2016 (4hours).
- 6) Iris Boccalero is born on 16th April 2016.
- 7) European Patent application No. 17170190.7 – 1607, "Method and systems for generating Electrical Energy, and sensor unit using them" by Boccalero and Boragno, has been approved on 30th June 2017.



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

Curriculum: Pharmaceutical, Food and Cosmetic Sciences

Daniele Brignole

Start of the Doctorate Program *November 1st, 2014*

End of the Doctorate Program *October 31st, 2017*

Advisors

Prof. Vincenzo Minganti

Prof.ssa Giuliana Drava

Report on research activity carried out during **the three years** of the course (01/11/2014-31/10/2017)

Thesis Title

Use of tree bark to study the distribution and concentration of trace elements in the atmosphere

Thesis abstract

The project is mainly focused on the study of the distribution and concentration of trace elements in the atmosphere, using vegetal bio-indicators such as tree bark. A bio-indicator is an indicator or part of it in which the concentration of a specific element reflects the concentration of the same element in the atmosphere.

The atmosphere itself is one of the powerful way by which the trace elements can be spread over long distances, depending on the time they remain suspended in it (considering an average time of 5 days). Because of their small dimensions (0.0005-100 μm) and the possibility of dispersion over long distances they can be a serious problem for the environment and for the human health.

To study the concentration of such elements in bio-indicators we have to consider two main pathways of deposition: wet deposition and dry deposition.

The wet deposition occurs during period of rain when the drops of water englobe the elements, present as "atmospheric particulate", and take them to the ground, while the dry deposition depends essentially on the sedimentation law and therefore on the dimension of the particulate.

The increasing focus on problems such as the traffic pollution and pollution related to industrial activities makes this project interesting because by a cheap and widespread indicator we would map and determine the concentration and distribution of several pollutants. Another important application is to analyze the increase of "emerging contaminants" such as the rare earth elements (REE), which are becoming more and more used in the industrial activities gaining an important role in new technological applications; therefore it would be useful to monitor these "new" elements and their impact on environment and human health.

ACTIVITY REPORT

Research Activity

Research Period Abroad

- 1) A **three month** research period, **08/01/2016 – 08/04/2016 (ERASMUS+ grant holder)** was carried out at the *Faculty of Science of the University of Lisbon (Portugal)*.
- 2) A **three-week** period, **20/06/2016- 11/07/2016**, was carried out at the Department of *Bioscience Engineering of the University of Antwerp (Belgium)*.

Scientific Publications

- 1) **Urban and industrial contribution to trace elements in the atmosphere as measured in holm oak bark.** *Giuliana Drava, Daniele Brignole, Paolo Giordani, Vincenzo Minganti, Atmospheric Environment (2016) 144, pp. 370-375*
- 2) **Branch bark of holm oak (*Quercus ilex* L.) for reconstructing the temporal variations of atmospheric deposition of hexavalent chromium.** *Giuliana Drava, Marco Anselmo, Daniele Brignole, Paolo Giordani, Vincenzo Minganti Chemosphere 170 (2017), 141-145*
- 3) **The bark of the branches of holm oak (*Quercus ilex* L.) for a retrospective study of trace elements in the atmosphere** *Giuliana Drava, Daniele Brignole, Paolo Giordani, Vincenzo Minganti, Environmental Research 154 (2017), 291-295*
- 4) **Is there a risk of trace element contamination in herbal preparations?** *Paolo Giordani, Vincenzo Minganti, Daniele Brignole, Paola Malaspina, Laura Cornara, Giuliana Drava Chemosphere 181 (2017) 778-785*
- 5) **Chemical and magnetic analyses on tree bark as an effective tool for biomonitoring: a case study in Lisbon (Portugal).** **Daniele Brignole** , Giuliana Drava, Vincenzo Minganti , Paolo Giordani , Roeland Samson , Joana Vieira , Pedro Pinho, and Cristina Branquinho **submitted to Chemosphere**

Communications at Conferences

Oral communications:

- 1) **Trace element bio-concentration and translocation in the edible medicinal herb *Plantago lanceolata***
Paolo Giordani, Giuliana Drava, Vincenzo Minganti, Daniele Brignole, Ilaria Ferretti, Paola Malaspina, Laura Cornara. SYRP: S.I.FIT. YOUNG RESEARCHERS PROJECT Siena, 19 February 2016
- 2) **Branch bark of trees as a viable approach for monitoring time variation of pollutants**
Brignole Daniele Workshop “La Giornata della Chimica Ligure: *Le attuali tendenze della ricerca chimica in Liguria*” Venerdì 20 Ottobre 2017 Presso DIFAR - Dipartimento di Farmacia, Viale Benedetto XV, 3 - Genova. Aula A

Poster Communications:

- 1) **Cobalt in bark of holm oak (*Quercus ilex* L.) in urban environments**
Daniele Brignole, Vincenzo Minganti, Paolo Giordani, Paola Malaspina, Giuliana Drava, EMEC 16 Torino, November 30th – December 3rd 2015

- 2) **Annual variations in trace element levels in the atmosphere as detected in holm oak bark of branch sections.**
Daniele Brignole, Giuliana Drava, Paolo Giordani, Vincenzo Minganti EMEC17 – 17th European Meeting on Environmental Chemistry – Inverness 30 Nov-2 Dec 2016
- 3) **Trace elements in a bioindicator and PM10: are they correlated?**
Daniele Brignole, Vincenzo Minganti, Paolo Giordani^a, Giuliana Drava
XXVI Congresso Nazionale della Società Chimica Italiana – Paestum 10-14/09/2017

Congresses Attended

- 1) 16th European Meeting on Environmental Chemistry (EMEC16) Torino, November 30th – December 3th 2015
- 2) 17th European Meeting on Environmental Chemistry (EMEC17) Inverness (Scozia), November 30th – December 2th 2016
- 3) XXVI Congresso Nazionale della Società Chimica Italiana – Paestum (SA) 10-14/09/2017

Courseware

Courses attended and passed (12 credits)

Courses Given by Teachers of the University of Genoa and IIT:

- 1) **Analisi multivariata dei dati chimici.** Docenti: Lanteri, Armanino, Leardi (**3CFU**); tenuto al Dipartimento di Farmacia, viale Brigata Salerno 13
- 2) **Marker molecolari della qualità e della genuinità degli alimenti** Docenti: Boggia, Zunin (**2CFU**); tenuto al Dipartimento di Farmacia, viale Brigata Salerno 13
- 3) **Biotecnologie farmaceutiche** Docente: Mazzei (**3CFU**); tenuto al Dipartimento di Farmacia, viale Benedetto XV, 3
- 4) **Metodi di preparazione e controllo di forme farmaceutiche innovative.** Docenti: S. Baldassari, G. Caviglioli, B. Parodi, E. Russo, G. Zuccari. (**2CFU**) tenuto al Dipartimento di Farmacia, viale Cembrano 4
- 5) **Tecniche strumentali per la determinazione di elementi in traccia di interesse farmaceutico, alimentare, ambientale.** Docenti: V. Minganti, G. Drava (**2CFU**) tenuto al Dipartimento di Farmacia, viale Cembrano 4

Courses Given by invited experts (5 credits):

- 1) **Solid State Modification: Principles and Applications for Drug Solubility Enhancement.**
Dr. Gatti venerdì 7 novembre 2014, aula B del Dipartimento di Farmacia, polo di Sturla via Brigata Salerno 13
- 2) **New trends in Computer aided drug design**
Prof. Tiziano Tuccinardi (Università degli Studi di Pisa e Adjunct Assistant Professor, Sbarro Institute for Cancer Research and Molecular Medicine Center for Biotechnology, Temple University, Philadelphia)
Martedì 11 Novembre 2014 presso Aula Angelo Ranise, DIFAR, S. Martino, Viale Benedetto XV, 3
- 3) **X-ray based experimental techniques and characterization of nano-material**
Dr. Alberto Morgante, CNR-IOM and Physics Department Trieste University, 31 marzo 2015 DCCI Aula 6

4) **Yb and Eu Strongly Correlated Electron Systems: from Experiment to Interpretation of Physical Properties**

Dr. Ivan Curlik, (University of Presov, Slovacchia), 21 e 22 Aprile 2015 presso le Aule 5 e 9 del DCCI, Via Dodecaneso

5) **Elementi di Chimica Forense**

Dott. Narizzano Riccardo e Dott.ssa Riso Fulvia, ARPAL, Genova,
Lunedì 18 Maggio presso l'aula 3 del DCCI e Martedì 19 Maggio presso l'aula 1 del DCCI

National and International Schools or Workshops

- 1) **Scuola di Chemiometria**, tenuta dal Gruppo di Chimica Analitica e Chemiometria della Sezione di Chimica e Tecnologie Farmaceutiche e Alimentari del Dipartimento di Farmacia dell'Università degli studi di Genova, Via Brigata Salerno 13 del Dipartimento di Farmacia, **Genova 25-28 Maggio 2015**
- 2) **Scuola di Experimental Design**, organizzata dal Gruppo di Chimica Analitica e Chemiometria della Sezione di Chimica e Tecnologie Farmaceutiche e Alimentari del Dipartimento di Farmacia dell'Università degli studi di Genova, Via Brigata Salerno 13, tenuta dal Prof. Riccardo Leardi, **Genova 21-25 Settembre 2015**
- 3) **3MS Envi School**, tenuta da Cecilia Bergamini (ARPA Emilia Romagna –Bologna), Rino Calori (ARPA Emilia Romagna –Bologna), Manuela Di Giovanni (ARPA Emilia Romagna –Bologna), Maria Ferrari (ARPA Emilia Romagna –Bologna), Gianluca Giorgi (Università di Siena) presso ARPAE Emilia Romagna, Via Francesco Rocchi, 1940138 **Bologna 19-20 Settembre 2017**
- 4) **Workshop “La Giornata della Chimica Ligure: Le attuali tendenze della ricerca chimica in Liguria”**
Venerdì 20 Ottobre 2017 Presso DIFAR - Dipartimento di Farmacia, Viale Benedetto XV, 3 - Genova. Aula A

Seminars Given

- 1) **Chronic Obstructive Pulmonary Disease (COPD): a pathology overview and the possible effects of Particulate Matter (PM)**
Dr. Brignole Daniele, Seminari SFAC 3 anno mercoledì 18 ottobre in AULA B, Difar, sezione Chimica del Farmaco e del Prodotto Cosmetico 14.30

Seminars Attended

- 1) **Biocatalisi: applicazioni in sintesi farmaceutica** *Dr. Matteo Massa*. Venerdì 28 novembre 2014
ore 14:30 presso il DiFar (sede di S. Martino) aula A. Ranise Viale Benedetto XV
- 2) **Molecole naturali e Xeno-ormesi** *Dr Giacomo Mele*. Venerdì 28 novembre 2014 ore 14:30 presso il DiFar (sede di S. Martino) aula A. Ranise Viale Benedetto XV
- 3) **Metodi alternativi alla sperimentazione animale** *Dr.ssa Benedetta Pollarolo*. Venerdì 28 novembre 2014 ore 14:30 presso il DiFar (sede di S. Martino) aula A. Ranise Viale Benedetto XV
- 4) **Recenti aspetti d'interesse terapeutico del processo di metastasi tumorale** *Dr.ssa Camilla Zibana*. Venerdì 28 novembre 2014 ore 14:30 presso il DiFar (sede di S. Martino) aula A. Ranise Viale Benedetto XV
- 5) **Ciclo di seminari su Assegni di Ricerca Po Cro FESR Liguria 2007-2013 Asse IV “Capitale Umano” relatori vari**. Giovedì 19 febbraio 2015 ore 09.00, Dipartimento di Chimica e Chimica Industriale, Aula Magna.
- 6) **Metabolomics Profile of Hypoxic Colorectal Cancer Cells** *Dr. PhD Alessandro Valli* (Research Scientist Weatherall Institute of Molecular Medicine, University of Oxford, UK). Venerdì 8 Maggio 2015 ore 14:30, presso il DiFar (sede di S. Martino) aula A. Ranise Viale Benedetto XV

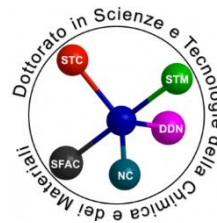
- 7) **Modelli per lo studio in vitro del metabolismo umano** *Prof. Arti Ahluwalia* Professore Associato di Bioingegneria Industriale, Dipartimento di Ingegneria dell'Informazione Università degli Studi di Pisa, Giovedì 16 luglio 2015 ore 15:00 Aula 3 Polo Alberti di Via L. B. Alberti 4
- 8) **The Biotin-(Strept)avidin system in pretargeting and in biotechnological applications**, *Dott.ssa Irene Croce* Venerdì 27 novembre 2015 ore 14.30 presso aula A. Ranise del DiFar (sede di S. Martino) Viale Benedetto XV, 3 Edificio n. 10, Genova
- 9) **Advanced technologies for the development of physiologically relevant in vitro alternative models**, *Dott.ssa Jenia Danailova* Venerdì 27 novembre 2015 ore 14.30 presso aula A. Ranise del DiFar (sede di S. Martino) Viale Benedetto XV, 3 Edificio n. 10, Genova
- 10) **Palladium-catalyzed reactions: a revolutionary impact in Medicinal Chemistry**, *Dott. Andrea Desogus* Venerdì 27 novembre 2015 ore 14.30 presso aula A. Ranise del DiFar (sede di S. Martino) Viale Benedetto XV, 3 Edificio n. 10, Genova
- 11) **Revolution in the treatment of parasitic diseases: Artemisinin as great scientific goal**, *Dott.ssa Cinzia M. Francini* Venerdì 27 novembre 2015 ore 14.30 presso aula A. Ranise del DiFar (sede di S. Martino) Viale Benedetto XV, 3 Edificio n. 10, Genova
- 12) **Druglikeness and related scoring methods: Ligand Efficacy and Lipophilic Ligand Efficacy** *Dott.ssa Sara Guariento* Venerdì 27 novembre 2015 ore 14.30 presso aula A. Ranise del DiFar (sede di S. Martino) Viale Benedetto XV, 3 Edificio n. 10, Genova
- 13) **Multi-block regression and classification based on PLS regression and extensions** *Prof. Tormod Naes* (Nofima, Ås, Norvegia ed Università di Copenhagen, Danimarca)_Lunedì 23 Maggio 2016 ore 14.30, Dipartimento di Farmacia, Viale Cembrano 4, Aula C
- 14) **Odori, profumi e feromoni come mediatori chimici olfattivi** *Dr.ssa Chiara Lacapra* 18 novembre 2016 ore 14.30 Dipartimento di Farmacia viale Benedetto XV Aula B
- 15) **Tubercolosi ed altre patologie polmonari: stato dell'arte e recenti sviluppi terapeutici** *Dr.ssa Elda Meta* 18 novembre 2016 ore 14.30 Dipartimento di Farmacia viale Benedetto XV Aula B
- 16) **Giocare sporco: PAINS e composti promiscui** *Dr.ssa Anita Parricchi* 18 novembre 2016 ore 14.30 Dipartimento di Farmacia viale Benedetto XV Aula B
- 17) **Il marketing cosmetico: dalla mission aziendale alla risposta del consumatore** *Dr.ssa Silvia Rum* 18 novembre 2016 ore 14.30 Dipartimento di Farmacia viale Benedetto XV Aula B
- 18) **The vaccines: from the origins to the present day** *Dr.ssa Monica Sanna* mercoledì 18 ottobre in AULA B, Difar, sezione Chimica del Farmaco e del Prodotto Cosmetico, ore 14.30
- 19) **Imaging in Oncology** *Dr.ssa Sara Pastorino* mercoledì 18 ottobre in AULA B, Difar, sezione Chimica del Farmaco e del Prodotto Cosmetico, ore 14.30
- 20) **Depression: new therapeutic strategies.** *Dr. Mohamed Sadeghi* mercoledì 18 ottobre in AULA B, Difar, sezione Chimica del Farmaco e del Prodotto Cosmetico, ore 14.30
- 21) **Probiotics: properties, uses and interaction with human gut microbiome** *Dr.ssa Federica Turrini* mercoledì 18 ottobre in AULA B, Difar, sezione Chimica del Farmaco e del Prodotto Cosmetico, ore 14.30

Other Activities

- 1) **Tutor didattico**, a.a 2015/2016 Chimica generale ed inorganica (59 ore), svolto per corso di Laurea Magistrale in Farmacia e corso di Laurea Magistrale in CTF
- 2) **Assistenza nei laboratori**, Analisi dei medicinali I (Far LM) 60 ore a.a 2015/2016 primo semestre (a partire dal 6/10/15)
- 3) **Tutor didattico**, a.a 2016/2017 Chimica generale ed inorganica (55 ore), svolto per corso di Laurea Magistrale in Farmacia e corso di Laurea Magistrale in CTF
- 4) **Assistenza nei laboratori** per l'insegnamento di Analisi dei Medicinali I per il corso di L.M. in Farmacia (40 ore) a.a 2016/2017 a partire dal 04/10/16 (primo semestre)



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



Curriculum: Science and Technologies of Materials

PAOLO - CANEPA

Start of the Doctorate Program *November 1st, 2014*

End of the Doctorate Program *October 31st, 2017*

Advisors

Prof.ssa Cavalleri Ornella

Thesis Title

Preparation, characterization and functionalization of Titanium Dioxide layer for biomedical applications

Thesis abstract

The project is centered on preparation and characterization of Titanium dioxide layers via anodization: the goal is to enhance the osteointegration and the biocompatibility of Titanium. For this purpose I'll also use the self assembly technique to have functionalized monolayers upon the Titanium surface.

ACTIVITY REPORT

Research Activity

Scientific Publications

- 1) ***"Phosphonate-anchored molecular layers on TiO₂ surfaces"*** (P. Canepa, I. Solano, S. Uttyia, G. Gemme, R. Rolandi, M. Canepa, O. Cavalleri) - MATEC web of conferences

Communications at Conferences

- 1) "Deposition of organic molecules bearing a phosphonate head group on TiO₂ surfaces" (ECOF 15 - poster)
- 2) "Functionalization of TiO₂ surfaces through phosphonate-anchored molecular layers" (N.I.C.E. 2016 - poster)

Congresses Attended

- 1) Misfolding proteico e amiloidosi XII
- 2) ECOF 15 – 15TH European Congress on Organised Films
- 3) N.I.C.E. 2016 – The 13TH International Conference on Bionspired and Biobased Chemistry & Materials

Courseware

During this 3RD year I have acquired **8** credits of Courseware.

Courses Given by Teachers of the Unige and IIT:

- 1) Basic Scanning and Transmission Electron Microscopies, Riani (3 credits)
- 2) Nanoparticle characterization by AFM and DLS, Rolandi (2 credits)
- 3) Metodi Ottici e Spettroscopici, Canepa, (3 credits)



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

Curriculum: Nanochemistry

MARCO CASSANI

Start of the Doctorate Program *November 1st, 2014*

End of the Doctorate Program *October 31st, 2017*

Advisors

Dr. Teresa Pellegrino (IIT), Prof. Gabriele Caviglioli (UniGe)

Thesis Title: “Iron oxide nanocubes as a platform for tumor targeting, oxaliplatin delivery and magnetic hyperthermia”

Thesis abstract

Introduction

Nanotechnology offers the possibility to exploit and modulate materials' properties at the nanoscale providing sustainable and effective cancer therapies. Nowadays, combinatorial therapies (*i.e.* chemotherapy with radiotherapy, combinatorial anti-tumoral drugs, hyperthermia with chemotherapy, *etc.*) are preferably used as clinical treatment against cancer. However, the development of a nanotool gathering different therapeutic properties is still challenging. Here, we propose iron oxide nanocubes (NCs) as a platform for developing a tumor selective and multi-responsive nanosystems to achieve multimodal strategy to treat cancer. We here exploit the very high heat performance of the nanocubes to perform magnetic hyperthermia. At the same time, the high surface area available of the nanocube has been used for drug delivery and specific antibody-mediated tumor targeting towards ovarian cancer cells.

Methods

We have chosen iron oxide nanocubes of 14 nm in cube edge because of their outstanding specific absorption rate (SAR) values under clinical conditions and under viscous environment such as that of tumors and cells. After their water transfer *via* a polymer coating procedure, the NCs were functionalized with an oxaliplatin-derived PEG (PEG-Pt) and a PEG-Bis(carboxymethyl)-lysine (a nitrilotriacetic derived molecule) complex for the binding of an his-tag antibody fragment (scFv) against folate receptor α (α FR). The presence of platin was assessed *via* ICP-AES and the presence of the antibody fragment on the nanocube was confirmed *via* SDS-PAGE, BCA and dot blot assays. The specificity of the nanocube binding was evaluated *via* flow cytometry by comparing the targeting efficiency of nanocubes modified with and without the scFv fragments towards tumor cell lines having different expression of α FR. Cytotoxicity of platin-modified nanocubes was assessed *via* presto blue and LDH assays. Finally, the contribution to the cytotoxicity provided by the magnetic hyperthermia treatment in combination or in absence of platinum cytotoxicity was also evaluated for nanocube samples bearing the antibody fragments and functionalized with or without the platin compounds.

Results

The targeting scFv protein fragments bound to the nanocube surface were active against α FR and provided specificity for accumulation toward ovarian cancer cell lines. While the scFv-modified nanocubes are biocompatible and non-toxic, they express severe toxicity when functionalized also with the oxaliplatin-derived PEG compound. Interestingly, the toxicity was higher in the cell lines positive for the expression of the α FR, compare to the negative ones. Furthermore, the hyperthermia treatment was observed to increase the toxicity of dual functionalized scFv platinum-modified nanocubes.

Conclusions

The bioconjugation strategy here chosen delivers iron oxide nanocubes functionalized with oxaliplatin-based drug and scFv antibody fragment. The nanocubes were able to induce tumor cytotoxicity mediated by oxaliplatin, based on the intracellular pH-release of the platinum ions. The targeting moieties (scFv) directed the toxicity specifically against the ovarian cell line. Moreover, magnetic hyperthermia further enhanced the nanocubes toxicity. Thus, combining drug delivery, targeting and magnetic hyperthermia nanocube's mediated, we developed a platform suitable for multitherapy against cancer.

ACTIVITY REPORT

Research Activity

The research activity was carried out at the IIT.

Conferences Attended

- 1) Nanomedicine symposium CEN@Regione Lombardia: "Synthesis of nanomaterials, biological applications and modelling", Milan 21 September, 2015.
- 2) ICONAN 2016, International conference on Nanomedicine and Nanobiotechnology, Paris 28-30 September 2016.
- 3) ANNIC 2017, International conference on Applied Nanotechnology and Nanoscience, Rome 18-20 October 2017.

Scientific Publications

Original publications on ISI Journals:

1) Facile transformation of FeO/Fe₃O₄ core-shell nanocubes to Fe₃O₄ via magnetic stimulation.

Lak A, Niculaes D, Anyfantis GC, Bertoni G, Barthel MJ, Marras S, Cassani M, Nitti S, Athanassiou A, Giannini C, Pellegrino T. *Sci Rep.* 2016 Sep 26;6:33295. doi: 10.1038/srep33295.

2) Multilayered Magnetic Nanobeads for the Delivery of Peptides Molecules Triggered by Intracellular Proteases. Alessandra Quarta, Marina Rodio, Marco Cassani, Giuseppe Gigli, Teresa Pellegrino, and Loretta L. del Mercato *ACS Appl. Mater. Interfaces* 31 Aug 2017 DOI: 10.1021/acsami.7b05709.

Courseware

During his PhD Marco Cassani has acquired **16 credits** of Courseware.

Courses Given by Teachers of the IIT Nanochemistry department:

- 1) Nanomaterials and Nanocomposites: Processing and characterization (7 hours) January 25th-February 15th, Dr. Luca De Trizio; Dr. Milena Arciniegas; Dr. Vladimir Lesnyak (**1 credits**)
- 2) Opto-Electronic Properties of Semiconductor Quantum Dots (7 hours) February 16th-March 10th, Dr. Iwan moreels (**1 credit**)
- 3) Characterization of functionalized and water soluble nanoparticles (7 hours) April 1st-April 25th, Dr. Teresa Pellegrino, Dr. Markus Barthel (**1 credit**)
- 4) Basics of Crystallography (7 hours) April 26th-May 21th, Dr. Liberato Manna (**1 credit**)

- 5) Electron microscopy (7 hours) June 11th-June 31st, Dr. Rosaria Brescia; Dr. Roberto Marotta (**1 credit**)
- 6) “Magnetic properties and characterization techniques” Aidin Lak, October 2015 (**1 credit**).
- 7) “Spectroscopies for chemical analysis (7 hours)” *Francisco Palazon* (Introduction to X-ray Photoelectron Spectroscopy), *Roman Krahn* (Introduction to Raman), *Sandeep Ghosh* (Introduction to NMR), October 2016 (**1 credit**).

Course Given by Teachers of the IBF-CNR (Type B):

- 1) Corso avanzato di dinamica molecolare di proteine, Dr. Oscar Moran (**3 credits**)

Course Given by Teachers of the DCCI (Type B):

- 2) Materiali magnetici funzionali, Prof. Fabio Canepa (**2 credits**)

Courses Given by invited experts (Type A):

- 1) “X-ray based experimental techniques and characterization of nano-materials” Alberto Morgante, CNR-IOM and Physics Department Trieste University, March 31st 2015, h. 14,30 – 17,30 DCCI Aula 6. (**1 credit**)
- 2) “Yb and Eu s correlated electron systems” Dr. Ivan Curlik, University of Presov, Slovacchia April 21st-22nd 2015, h. 10,00 – 12,30 DCCI Aula 5 e 9. (**1 credit**)
- 3) “Magnetic hyperthermia: from fundamentals to biological applications” Francisco Teràn, iMdea Nanociencia, Ciudad Universitaria de Cantoblanco, Madrid, Spain; May 5th-6th 2016 (**1 credit**).
- 4) “An introduction to nanoscale magnetism for biomedical applications” Speaker: Neil Telling, Keele University, UK, May 23rd-24th 2017 (**1 credit**).

Seminars Attended

- 1) “Materials for sodium batteries” Dr. Stefano Passerini, January 16th, 2015.
- 2) “Designing organometallics for material science: application for solar cells and scintillators” Dr. Guillaume Bertrand, January 19th, 2015.
- 3) “Design, fabrication and characterization of plasmonic structures for graphene-based devices and superresolution” Dr. Valeria Lotito, January 19th, 2015
- 4) “Using colloidal quantum dots to boost photovoltaic cell performance” Dr. Miri Kazes, February 25th, 2015.
- 5) “Versatile fabrication of highly porous cryogels from noble metal nanoparticles” Dr. Axel Freytag, March 04th, 2015.
- 6) “Structure activity relationship in CO oxidation over bimetallic AuCu nanocrystals: the role of nanocrystals size, composition and support interaction” Dr. Massimo Colombo, March 18th, 2015.
- 7) “Visualizing and controlling optoelectronic processes in lead halide perovskites” Dr. Alexander Weber-Bargioni, November 14th 2015.
- 8) “Semiconductor Nanocrystals: Discovery, Milestones, and Recent Theoretical Developments” Dr. Alexander L. Efros, November 20th, 2015.
- 9) “Hydration induced spin glass state in a frustrated Na-Mn-O triangular lattice” Dr. Ioanna Bakaimi, April 28th, 2016.
- 10) “Colloidal nanoparticles and application” Dr. Antonios G. Kanaras, April 28th, 2016.
- 11) “Thermal forces: Moving and manipulating matter with thermal gradients” Prof. Roberto Piazza, October 21st, 2016.
- 12) “NMR chemosensing with self-organized nanoparticles based receptors” Prof. Fabrizio Mancin, November 3rd, 2016.
- 13) “Biomolecule analytics using microscale thermophoresis (MST)” Dr. Francesca Viganò, November 10th, 2016.
- 14) “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, 28th February 2017.

- 15) "Synthetic methodology for colloidal nanomaterials: limitations and opportunities" Prof. Dmitri Talapin, Department of Chemistry and James Franck Institute, University of Chicago, 26th May 2017.
- 16) "The role of membrane curvature at the nano-bio interface" Prof. Bianxiao Cui, Department of Chemistry, Stanford university, CA, USA, 12th September 2017.
- 17) "Nanoparticles and viruses", Prof. Francesco Stellacci, EPFL, Lausanne Switzerland, 22nd September 2017.
- 18) "Standardization methods for the synthesis of single-core and multi-core magnetic nanoparticles for medical applications", Helena Gavilan Rubio - Instituto de Ciencia de Materiales de Madrid, ICMM/CSIC, Madrid, Spain, 3rd October 2017.

(2 credits in total)

Group meetings

- 1) NACH group meeting 17th December 2015, "Bioconjugation of magnetic nanoparticles for tumor targeting" **(1 credit)**
- 2) NABM group meeting 5th June 2017, 7th June 2017, "Bioconjugation of iron oxide nanocubes for a combinatorial therapy of cancer" **(1 credit)**.

National and International Schools or Workshops

- 1) Utrecht Summer School, summer program "Nanomedicine", 20th July-24th July 2015. **(1.5 ECTS)**
- 2) ERC "ICARO" Kick off meeting, Sestri Levante, 9th-10th June 2016 Oral presentation "Bioconjugation of magnetic nanobeads for tumor targeting" **(1 credit)**
- 3) ANNIC 2017, International conference on Applied Nanotechnology and Nanoscience, Rome 18-20 October 2017. Oral Presentation "Magnetic iron oxide nanoparticles for cancer treatment and diagnosis" **(1 credit)**



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

Curriculum: Nanochemistry

Andrea Castelli

Start of the Doctorate Program: 1st November 2014

End of the Doctorate Program: 31st October 2017

Advisors

Prof. F. Buatier de Mongeot (UniGe);
Prof. L. Manna and dr. M. P. Arciniegas (IIT)

Thesis Title

“Development and Analysis of Self-Assembled Structures of Nanocrystals”

Thesis abstract

In recent years remarkable scientific progress has been achieved in the development of synthetic protocols of nanomaterials, which has allowed access to a variety of shapes and sizes in colloidal nanocrystals (NCs). This has significantly impacted the development of hierarchically ordered structures, that involve the use of pre-existing NCs with well-defined shapes and monodispersed sizes, as a promising route to integrate NCs in microscale devices for many applications. Thus, great efforts has been devoted to the spontaneous organization of NCs, which can be seen as a powerful tool to achieve highly ordered nanostructures. While self-assembly of colloidal NCs with simple shapes (spheres, rods, disks) has been deeply investigated, the behaviour of particles with more elaborate geometries is still not fully understood. The goal of this PhD course was the fabrication, characterization and analysis of self-assembled structures made of anisotropic colloidal NCs, following a systematic and rationalized experimental approach. Here, different assembly techniques such as organic-induced, solvent evaporation, liquid interface-induced, among others, were exploited to control the aggregation phenomena of NCs that resulted into one-dimensional to three-dimensional structures. A detail analysis of relevant physicochemical parameters, such as,at the various stages of the nanolattice formation was conducted in order to elucidate the assembly mechanism of the different studied systems.

The first year of research activities was dedicated in particular to the development of 2D nanolattices built with two type of NC shape by using branched CdSe/CdS core/shell NCs and isotropic nanospheres. In this case a liquid-liquid interface strategy was used to investigate the formation of intercalated binary structures. The project started with the improvement on the synthesis of branched NCs that have eight CdSe pods that grow from a CdSe core (so named octapods), in order to achieve

control over their shape and size. Combining the so formed NCs with shape-complementary spheres and carefully tailoring the octapods aspect ratio and ligand shell, 2D ordered membranes can be obtained. They consist of mosaics of intercalated structures where octapods and spheres, in the projections given by electron microscopy investigation, are disposed following a “tic-tac-toe” arrangement, with octapods standing on four pods and one sphere is located in the empty volume created by the octapods’ convex geometry.

The second year of PhD was focus on two different projects:

- i) Starting from the results obtained in the first year, a methodical investigation of the self-assembly behaviour of octapods 2D membranes formed by particles of different dimensions and with different ligand shells was conducted. This led to the definition of a concentration/size phase diagram that can be divided in particles forming interlocked and non-interlocked membranes, to identify a strong inhomogeneity in the ligand shell of the particles and to highlight its fundamental role in dictating the final geometry of the assembled structure. Indeed, by FTIR analysis of octapods surface, we demonstrated the presence of a cone-like distribution of ligands, giving a thicker shell toward the tips and, thus, an inhomogeneous interaction of the pod with other pods. Experimental and numerical simulations showed that this ligand distribution is responsible for the interlocking of octapods in chains and that, by proper ligand exchange, several different self-assembly configurations can be obtained.
- ii) The behaviour of octapods when assembled starting from a mixture with polystyrene (PS) in solution was deeply investigated, and it showed that the NCs preserve their tendency to form interlocked chains, in this case, within a free-standing polymer film. By providing thermal energy to the resulting composite film, the linear arrays of octapods gain mobility and formed longer structures by a tail-to-tail coupling. Given the thickness of the composite the presence of the chains could not be verified via electron microscopy investigation, but confocal nonlinear spectroscopy was instead employed, exploiting the tenuous emission arising from CdS pods. Finally, the mechanical properties of the composite film were studied via creep tests at 70°C. The results showed that there is an enhancement of over 30% of the creep modulus in the nanocomposite compared to pure PS thanks to the ability of self-assembled chains to anchor the polymer and prevent its slippage.

The third year was focused on octapods surface and shape modification with two main goals: i) to create 3D binary assemblies of octapods and cubes NCs, and ii) to produce highly anisotropic and fluorescent NCs to elucidate their geometry-related assemblies in 2D planar nanolattices. To reach the first goal of this last year, there was the need to impose to both components (octapods and cubes) a strong mutual surface recognition tool. Shape complementarity was found not to be enough for these NCs to interact. The particles, thus, were transferred into polar phase to exploit electrostatic attraction. For the water transfer of octapods small molecules (mercaptopyropionic acid – MPA, dopamine – DOP and mercaptopropanesulfonic acid – MPS) were successfully employed, allowing ζ -potential tuning (negative for the acids and slightly positive for the amine). In contrast to the ones precipitated from toluene suspensions, the transferred octapods do not aggregate in interlocked chains, forming instead porous structures. On the other hand, cube NCs were transferred into water by using a well-established polymer coating with functionalized poly(ethyl glycol). When cubes were added to the octapod solution, the resulting co-aggregates show phase segregation. We ascribed cubes segregation to an intercalation of polymer chains that makes cube-cube interactions more favourable than cube-octapod interactions. In order to overcome this issue we started a collaboration with dr. Pellegrino and dr. Mai aiming the introduction of a similar polymer coating on the octapods. Preliminary results show excellent stability in water for polymer-coated octapods and a marked tendency to create tip-to-tip contact, leaving empty pockets able to host the cubes.

In order to obtain fluorescent branched NCs, the Cu_{2-x}Se seeds employed in the octapods synthesis had been replaced by green emitting zinc-blende CdSe platelets. The new syntheses resulted in bone-shaped nanoparticles (nBones) with four pods at each end of a platelet-like body. The pods are formed by wurtzitic CdS, while the body by zinc-blende CdS, signalling that the original platelets underwent anion exchange. Moreover, depending on their length, the pods modifies their geometry, switching

from tetrahedral (short pods) to octapod-like (long pods). The particles lost the quantum well-like emission of the starting seeds, but retained a red luminescence (max at 660 nm) that can be ascribed to CdSe quantum dots embedded in the structure. This emission (maximum photoluminescence quantum yield, PLQY, of 10%) is stronger than what observed from octapods and decreases its intensity in particles with longer pods. Similar trend can be observed in two absorption peaks (500 nm and 550 nm) that can also be ascribed to the presence of excitons confined in CdSe QDs. The presence of Se in the structure was furtherly verified by energy dispersive X-ray spectroscopy. Preliminary assembly experiments showed that nBones own a wide self-organization versatility as they are able to create different configurations such as ribbons and herring-bone in their planar nanolattices.

ACTIVITY REPORT

Research Activity

The research activity was mainly carried out at the IIT facilities in via Morego, 30 - Genova.

Scientific publication

- 1) Castelli A. et al., *Tic-Tac-Toe Binary Lattices from the Interfacial Self-Assembly of Branched and Spherical Nanocrystals*, ACS Nano 2016, **10**: 4345-4353
- 2) Arciniegas M. P., Castelli A. et al., *Assembly of Branched Colloidal Nanocrystals in Polymer Films Leads to Enhanced Viscous Deformation Resistance*, Nano Letters 2016, **16**(10): 6154-6163.
- 3) Arciniegas M. P., Castelli A. et al., *Laser-Induced Localized Growth of Methylammonium Lead Halide Perovskite Nano- and Microcrystals on Substrates*, Advanced Functional Materials 2017, **27**(34): 1701613-n/a.
- 4) Castelli A. et al., *Understanding and Tailoring Ligand Interactions in the Self-Assembly of Branched Colloidal Nanocrystals into Planar Superlattices*, Nature Communications, Under 1st revision.

Communications at Conferences

Oral contributions:

- 5) *"Tic-Tac-Toe Binary Lattices from the Interfacial Self-Assembly of Branched and Spherical Nanocrystals"*. 252nd American Chemical Society National Meeting & Exposition, 21st – 25th August 2016, Philadelphia, USA. It received the award for the "Best presentation of the session";
- 6) *"Synthesis and Self-Assembly of Emitting Bone-Shaped Colloidal Nanocrystals"*. 3rd International Conference on Nanomaterials: Fundamentals and Applications. 9th – 11th October 2017. Štrbské Pleso, Slovakia.

Poster Communications:

- 7) *"Self-Assembly of Octapod-shaped Colloidal Nanocrystals into a Hexagonal Ballerina Network Embedded in a Thin Polymer Film"*. 14th European Conference on Organized Films. 29th June – 2nd July 2015. Genoa, Italy;
- 8) *"Tuning Particle Interactions of Branched-Shaped Nanocrystals Toward Control over 2D Self-Assembled Superstructures"*. Nanoparticles with Morphology and Functional Anisotropy – Faraday Discussion. 4th – 6th July 2016. Glasgow, Scotland;

- 9) *"A View on the Self-Assembly of Colloidal Branched Nanocrystals"*. 11th International Summer Schools on N&N, Organic Electronics & Nanomedicine (ISSON17). 1st – 8th July 2017, Thessaloniki, Greece;

Participation in Congresses

1. ECOF – 14, 14th European Conference on Organized Films. 29th June – 2nd July 2015. Genoa, Italy;
2. Nanoparticles with Morphology and Functional Anisotropy – Faraday Discussion. 4th – 6th July 2016. Glasgow, Scotland;
3. 252nd American Chemical Society National Meeting & Exposition 21st – 25th August 2016. Philadelphia, USA;
4. 3rd International Conference on Nanomaterials: Fundamentals and Applications. 9th – 11th October 2017. Štrbské Pleso, Slovakia.

Courseware

During the 3 years Andrea Castelli has acquired 20.875 credits of Courseware.

Courses attended and passed (15 credits):

- 1) "Nanomaterials and Nanocomposites: Processing and characterization"
Dr. De Trizio L., Dr. Arciniegas M., Dr. Lesnyak V. (28 February and 3, 5 March 2015, IIT) – 1 credit.
- 2) "Opto-Electronic Properties of Semiconductor Quantum Dots"
Dr. Moreels I. (18, 24 February and 3, 10 March 2015, IIT) – 1 credit.
- 3) "Energy storage and catalysis"
Dr. Colombo M., Dr. Monaco S. (17, 19, 24, 26 March 2015, IIT) – 1 credit
- 4) "Characterization of functionalized and water soluble nanoparticles"
Dr. Pellegrino T., Dr. Barthel M., Dr. Lesnyak V. (10, 14, 17, 21, 27 April 2015, IIT) – 1 credit.
- 5) "Basics of Crystallography"
Prof. Manna L. (29 April and 5, 12, 19 May 2015, IIT) – 1 credit.
- 6) "X-rays based Characterization Techniques"
Dr. Prato M., Dr. Palazon F. (22, 28 May 3, 9 June 2015, IIT) – 1 credit.
- 7) "Electron microscopy"
Dr. Brescia R., Dr. Marotta R. (16, 19, 25 June 2015, IIT) – 1 credit.
- 8) "Electrical and Raman characterization techniques"
Dr. Krahne R. (17-22-24 September 2015, IIT) – 1 credit.
- 9) "Magnetic properties and characterization techniques"
Dr. Lak A. (6-9-16 October 2015, IIT) – 1 credit.
- 10) "Electronic properties of solids"

Prof. Manna L. (2, 9, 16, 23 March, 1, 13, 20, 27 April, 4, 11, 16 May 2015, IIT) – 3 credits.

- 11) "Advanced Optical Fluorescence Microscopy Methods I"
Prof. Diaspro A. (29, 30, 31 May 2017, IIT) – 3 credits

Courses Given by invited experts (3 credits):

- 1) "Modern Materials for Energy Saving (Renewable Energy)", Prof. Peter Rogl, Institute of Physical Chemistry, University of Vienna, Austria (9 -10 June 2015, DCCI, Università di Genova) – 1 credit.
- 2) "Conventional and Unconventional Superconductivity: An overview", Prof. Ernst Bauer, Institute of Solid State Physics, Vienna University of Technology, Austria (9-11 November 2015, DCCI, Università di Genova) – 1 credit.
- 3) "Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials", Prof. Thomas Fässler, Department of Chemistry – Technical University of Munich, Germany (11 May 2017, DCCI, Università di Genova) – 1 credit

Seminars Attended (2.875 credits):

- 1) Plasencia J. I. C., "Optics of CdSe/CdS nanocrystals: a theoretical overview", IIT, 5/12/2014;
- 2) Garrido J. A., "CVD-based graphene field-effect transistors and electrodes", IIT 10/12/2014;
- 3) Mehdi H., "Plasmonic Nanomaterials", IIT, 12/1/2015;
- 4) Bertrand G., "Designing organometallics for material science: application for solar cells", IIT, 19/1/2015;
- 5) Lotito V., "Design, fabrication and characterization of plasmonic structures for graphene-based devices and superresolution", IIT, 19/1/2015;
- 6) Prato M., "Synergies between chemistry and nanotechnology: application to neurosciences and energy", IIT, 27/01/2015;
- 7) Konstantatos G., "Colloidal Quantum dot Optoelectronics: Photodetectors and solar cells", IIT, 30/1/2015;
- 8) Freytag A., "Versatile fabrication of highly porous cryogels from noble metal nanoparticles", IIT, 4/3/2015;
- 9) Colombo M., "Structure-activity relationship in CO oxidation over bimetallic AuCu Nanocrystals: the role of nanocrystal size, composition and support interaction", IIT, 18/3 2015;
- 10) Arnault J. C., "Control of surface chemistry of nanodiamonds for bio-applications", IIT, 9/11/2015;
- 11) Efros A. L., "Semiconductor Nanocrystals: Discovery, Milestones and Recent Theoretical Developments", IIT, 20/11/2015;
- 12) Reiss P., "Insight in the chemistry of metal sulfide nanocrystals and their application in photovoltaics", IIT, 25/11/2015;
- 13) Flatten L., "Recent advances with FIB-milled microcavities", IIT, 19/1/2016;
- 14) Perez L. M., "Perovskites: an old material for the third generation of PV solar panels", IIT, 21/4/2016;
- 15) Kanaras A. G., "Colloidal nanoparticles and applications", IIT, 28/4/2016;
- 16) Bakaimi I., "Hydration induced spin glass state in frustrated Na-Mn-O triangular lattice", IIT, 28/4/2016;

- 17) Cacialli F., "The power of intermolecular interactions in organic semiconductors: from threaded molecular wires to PCBM single crystals", IIT, 5/5/2016;
- 18) Basov D. N., "Nano-photonic phenomena in van der Waals heterostructures", IIT, 8/6/2016;
- 19) Armaroli N., "Photoactive Systems for Solar Energy Conversion, Luminescence and Catalysis", IIT, 27/1/2017;
- 20) De Angelis F., "Interplay of Electronic and Dynamical Processes in Organohalide Perovskites", IIT, 14/3/2017;
- 21) Amoroso S., "Theatrocracy: the communication in the modern age", IIT, 2/5/2017;
- 22) Talapin D., "Synthetic Methodology for Colloidal Nanomaterials: Limitations and Opportunities", IIT, 26/5/2017;
- 23) Chan E., "High-Throughput Design of Doped Colloidal Nanocrystals", IIT 1/6/2017;

National and International Schools or Workshop

1. D3 Workshop: "Cancer Stem Cells and Autophagy: Diagnostic and Drug Discovery". 27th March 2017, IIT Genoa, Italy;
2. 11th International Summer Schools on N&N, Organic Electronics & Nanomedicine (ISSON17). 1st – 8th July 2017, Thessaloniki ,Greece;

Other Activities

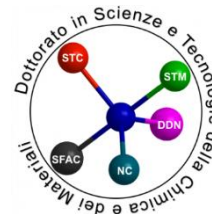
Publication of:

Castelli A. et al., *High-Efficiency All-Solution-Processed Light-Emitting Diodes Based on Anisotropic Colloidal Heterostructures with Polar Polymer Injecting Layers*, Nano Letters 2015, **15**(8): 5455-5464.1.



Università degli Studi di Genova

Doctorate School in Sciences and Technologies of Chemistry and Materials



Curriculum: Nanochemistry

Lin Chen

Start of the Doctorate Program *November 1st, 2014*

End of the Doctorate Program... *October 31st, 2017*

Advisors

Prof. Libero Manna (IIT); Dr. Simone Monaco (IIT); Bruno Scrosati (IIT); Marco Panizza (DICCA)

Thesis Title

The Investigation of Inorganic Nanocrystals Electrode Materials for Lithium and Sodium Ion Batteries

Thesis abstract

A promising way to reduce the diffusion pathway of Li-ion or Na-ion and consequently improve the charge/discharge electrochemical performances of LiMnPO_4 and $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ base cathodes is the use of nanoscale materials. My research of 1st year was mainly focused on: 1) the investigation of effective conductive carbon coating of LMP (LiMnPO_4) nanocrystals by etching the surface of the particles synthesized via colloidal, hydro and solvo-themal methods. A surface treatment with lithium hexafluorophosphate (LiPF_6) to remove the surfactant ligand shell of the LMP colloids samples was studied. The structure and morphology were still preserved after carbon coating. The initial charge-discharge, cycle and rate performances are obviously improved. It also applied to the samples prepared by hydrothermal and thermal. 2) the investigation of the synthesis procedure of LNMO ($\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$) nanoparticles and the study of their electrochemical performance in both lithium ion batteries. Pure LNMO ($\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$) nanoparticles were obtained by adding lithium salt to NMO sample before the pyrolysis process. The particles after heat treatment grow up and the electrochemical performances are worse than the references. What we want to improve is to control the size of the particles and substitute the Na for parts of Li in LNMO to improve the electrochemical by trying different methods to add the lithium salt.

My research of 2nd year was mainly focused on two parts. Firstly, followed the 1st years' work, I continued the study of $\text{Ni}_{0.25}\text{Mn}_{0.75}\text{O}$. In order to make the crystals hydrophilic and therefore allow an adequate mixing with the aqueous glucose solution, the aliphatic surfactants were removed by treating the NCs with an aqueous LiPF_6 solution, following the same etching procedure developed in our previous paper. The NiMn_2O_4 (NMO) and $\text{NiMn}_2\text{O}_4/\text{C}$ (NMO/C) pure phase were obtained after the pyrolysis. The electrodes were prepared and tested as anodes for LIBs and SIBs. Most of the efforts were on the second part, which is the study of the P2-type $\text{Na}_{1.7}\text{Ni}_{1.0}\text{Mn}_{2.9}\text{O}_{7.6}$ layered oxide as cathode material for the Na-ion battery. A two-step synthesis comprising a first colloidal step followed by a second sodiation step carried out *via* a solid state reaction was applied to get the material. By the adopted synthetic protocol and working at Na:Ni:Mn ratios of 1.7:1:3 we were able to produce a cathode material for Sodium-ion batteries that could withstand long charge/discharge cycles at working voltages up to 4.4 V vs. Na^+/Na .

For the 3rd year, I continued the study of the P2-phase NaNMO layered oxide as cathode for Na-ion batteries. The main problem of these materials is the poor structure stability upon the Na⁺ intercalation/deintercalation at high operating voltage as cathode material. When they are deeply charged, a low amount of the Na in the structure induced the gliding of the T_MO₆-layers, with the transition of O2-phase. The material couldn't cycled above 4.2 V (vs. Na⁺/Na) because of this P2-O2 phase transition is irreversible, which narrows the voltage window and limits the energy delivered. We use the colloidal+solid-state reaction to obtained the P2-phase NaNMO sample and the operando XRD measurements shows there's no P2-O2 phase transition even we charged the cell up to 4.4 V, which gives a good structure stability during cycling.

Inspired by this work, we started the study of another P2-phase materials, NaNTO. This Ni-containing layered oxide material, has been proved to function as both positive material with 90 mAh/g (x from 2/3 to 1/3) as well as negative material with 90 mAh/g (x from 2/3 to 1) for the Na-ion batteries by selectively activating the high voltage redox couple Ni²⁺/Ni⁴⁺ (3.5 V) or the low voltage couple Ti⁴⁺/Ti³⁺ (0.7 V). We studied the electrochemical performances of this materials as both cathode and anode material for Na-ion batteries. Besides, we tried to assemble the symmetric full cell with this bi-functional layered oxide material.

ACTIVITY REPORT

Research Activity

The research activity was mainly carried out at the IIT.

Scientific Publications

Original publications on ISI Journals:

- 1) Lin Chen, Enrico Dilella, Andrea Paoletta, Giovanni Bertoni, Alberto Ansaldo, Massimo Colombo, Sergio Marras, Bruno Scrosati, Liberato Manna*, and Simone Monaco*, *Relevance of LiPF₆ as Etching Agent of LiMnPO₄ Colloidal Nanocrystals for High Rate Performing Li-ion Battery Cathodes*, *ACS Appl. Mater. Interfaces*, 2016, 8, 4069-4075;
- 2) Lin Chen, Michele Fiore, Ji Eun Wang, Riccardo Ruffo, Do-Kyung Kim and Gianluca Longoni*, *Readiness level of Sodium-ion battery technology: a materials review*. [adsu.201700153](https://arxiv.org/abs/201700153);
- 3) Lin Chen, Sergio Marras, Giovanni Bertoni, Francisco Palazon, Mauro Gemmi Liberato Manna*, Simone Monaco*, *Colloidally Assisted Synthesis to Phase Pure Na_{1.7}Ni_{1.0}Mn_{2.9}O_{7.6} with Suppressed P2/O2 Phase Transition as High Stable Cathode for Na-ion Batteries*, submitted.

Courseware

During her 3 years, Chen Lin has acquired 28 credits of Courseware.

Courses attended and passed (21 credits)

Courses Given by Teachers of the IIT:

- 1) Opto-Electronic Properties of Semiconductor Quantum Dots -7 hours, Iwan Moreels (1 credit)
- 2) Energy Storage and Catalysis-7 hours, Massimo Colombo, Simone Monaco (1 credit)
- 3) Basic of Crystallography-7 hours, Liberto Manna (1 credit)
- 4) X-rays based Characterization Techniques -7 hours, Miko Prato(1 credit)
- 5) Electron Microscopy-7 hours, Rosaria Brescia, Roberto Marotta (1 credits)
- 6) Science and Technology of Two-Dimensional Crystals-7 hours, Francesco Bonaccorso (1 credit)
- 7) Electric Circuits For Electrochemistry-10 hours, Alberto Ansaldo, David Gendron (3 credits)

- 8) Characterization of Polymeric Materials, Luca Ceseracciu, Josè Guerrero (4 credits)
- 9) Electronic properties of solids- 22hours, Liberato Manna (3 credits)
- 10) Magnetic properties and characterization techniques-7 hours, Aidin Lak (1credit)
- 11) Nanomaterials and Nano-heterostructures: colloidal synthesis and chemical transformation- 7 hours, Luca De Trizio (1 credits)

Courses Given by invited experts: (Course A, B)

- 1) Green Analytical Chemistry Course-4 hours, Estrella Espada Bellido, DCCI, Università di Genova (1 credit)
- 2) Conventional and Unconventional Superconductivity: An overview-5 hours, Prof. Ernst Bauer, DCCI, Università di Genova (1 credit)
- 3) Basics in Electrochemistry -4 hours, Simone Monaco, Sebastiano Bellani and Haiyan Sun, IIT (1 credit)

National and International Schools, Workshops and conferences (1)

- 1) Attended the “Electrochemical Impedance Summer School Training” held at the Department of Chemistry, University of Bath, UK;
- 2) Research visit Nanoscience Laboratory at Aston University, Birmingham, UK;
- 3) Materials.it 2016, 12th -16th Dec. 2016, Catania, Italy;
- 4) 231st ECS (The Electrochemical Society) meeting, 28th May-1st June, 2017, New Orleans, LA, USA.
- 5) ANNIC 2017 (Applied Nanotechnology and Nanoscience International Conference 2017), 18th Oct.-20th Oct. 2017, Rome, Italy.

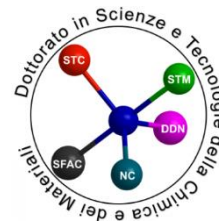
Seminars Given (4 credits)

- 1) The investigation of inorganic nanocrystals electrode materials as lithium and sodium ion batteries, Group meeting, IIT, 14/01/2016;
- 2) Introduction of Basic Electrochemical Cell and Lithium Ion Batteries, IIT, 23/06/2016;
- 3) Lithium ion batteries: Working Mechanism & Principle Configuration, IIT, 22/07/2016;
- 4) Lithium Ion Batteries: Electrodes of Lithium Ion Batteries, IIT, 29/07/2016.

Seminars Attended(2 credits)

- 1) High Energy Lithium-ion and Lithium-Sulfur Batteries, Marco Agostini, IIT, 20/2/2015.
- 2) Using colloidal quantum dots to boost photovoltaic cell performance, Miri Kazes, IIT, 25/02/2015.
- 3) Structure-activity relationship in CO oxidation over bimetallic AuCu Nanocrystals: the role of nanocrystals size, composition and support interaction, Colombo M., IIT, 18/03/2015.
- 4) Manufacturing, Manipulation and Measurement at Nanoscale with Femtosecond Laser Photons. Hong-bo Sun, IIT, 18/06/2015.
- 5) Synthesis and Chemical Manipulation of Nanoparticles for Magnetic Improvement, Dr. Verónica Salgueirino, IIT, 11/11/2015;
- 6) Semiconductor: Discovery, Milestones and Recent Theoretical Developments, Prof. Alexander L. Eforos, IIT, 20/11/2015;
- 7) Insight in the chemistry of the metal sulphide nanocrystals and their application in photovoltaics, Dr. Peter Reiss, IIT, 25/11/2015;
- 8) Materials for therapy: Cerium oxide nanoparticles as novel antioxidant drugs, Prof. Enrico Traversa, IIT, 03/02/2016;
- 9) Perovskites: an old material for the third generation of PV solar panels, Dr. Laura Miranda Perez, IIT, 21/04/2016;
- 10) Spatio-temporal visualization of atomic motions in low-dimensional materials, Dr. Giovanni Maria Vanacore, IIT, 03/05/2016;
- 11) The Power of Intermolecular Interactions in organic semiconductors: from threaded molecular wires to PCBM single crystals. Prof. Franco Cacialli, IIT, 05/05/2016;
- 12) First-Principles predictions of substrate effect on silicone, Prof. Udo Schwigenschloegl, IIT, 09/05/2016;
- 13) Nano-photonic phenomena in vander waals heterostructures, Prof. Dmitri N. Basov, IIT, 08/06/2016;
- 14) The Research Trend for the Next- Generation Rechargeable Batteries in Korea: A Perspective for Materials Design Approaches, Prof. KIM DO-KYUNG, IIT, 17/03/2017;

- 15) Combined TERS-STM characterization of self-assembled monolayers and micro-Raman of different nanomaterials, Chiara Toccafondi, iit, 12/04/2017.
- 16) Perovskite nanocrystals - the new generation of defect tolerant luminescent materials, prof. Sameer Sapra, iit, 14/06/2017.
- 17) The Electrochemical & Physical Performance Benefits of Graphene into Li-ion Energy Storage Technologies, Melanie Loveriduge, IIT, 15/09/2017.



Università degli Studi di Genova

Doctorate in Sciences and Technologies of Chemistry and Materials

Curriculum: XXX

Duc Anh Dinh

Start of the Doctorate Program November 1st, 2014

End of the Doctorate Program October 31st, 2017

Advisors: Dr Francesco Bonaccorso (IIT), Dr Vittorio Pellegrini (IIT), Prof. Paolo Piccardo (DCCI)

Thesis Title: Production of graphene and other 2D crystal-based functional electrodes for Li-ion batteries

Thesis abstract

The rapid development of electronic portable devices, electric cars, etc. has boosted the requirement of portable and efficient energy storage systems. In this context, lithium ion batteries (LIBs) technology has emerged as one of the most promising for these applications. Many efforts have focused on lithium ion batteries research and technology, achieving significant results. However, a critical challenge that LIBs technology is currently facing is the development of high-performance anodes, capable of yielding high specific capacity and energy efficiency, as well as long cycle life and low cost, in order to adapt to the environmental constraints and ultimately suit the needs of an industrial-scale production. Conventional LIB anodes are commonly based on graphite as active material. However, the main limiting factor of graphite relies on its theoretical maximum specific capacity that is limited to 372 mA h g^{-1} . For this reason, there is a huge scientific interest in replacing graphite with a higher specific capacity anode material. For example, metal and metal oxide, such as Sn, Sb, Si, Ge, SnO_2 , and Co_3O_4 , have been reported to possess higher lithium storage capacities (the theoretical capacity of Sn: 993 mA h g^{-1} , Si: 4200 mA h g^{-1}) than graphite via the formation of alloys with lithium or through the reversible reactions with Li^+ ions. However, these electrodes are still facing the issue associated with the huge volume variation during the charge/discharge cycles, resulting in the pulverization of the electrode, and consequently poor electrochemical reversibility. The idea about a new generation of LIBs with long lasting life cycles and high specific capacity is still a huge challenge for scientific community. Thus, seeking new materials for the next-generation of LIBs is a mandatory task for both research and industry.

The aim of my PhD work is to investigate nanomaterials, *e.g.*, carbon nanotubes (CNTs) as well as graphene and other two-dimensional (2D) crystals as potential materials for future LIB electrodes. In particular, I focused on the production of graphene- and molybdenum disulfide (MoS_2)-based inks. I investigated the role of the morphology of flakes in lithium ion storage capability of graphene-based anodes and the electrochemical activities of MoS_2 anodes.

Currently, commercial LIB anodes are based on graphite due to its high coulombic efficiency ($\sim 99\%$), low potential profile versus lithium ($\sim 0.2 \text{ V}$) and structural stability during charge/discharge cycling. However, graphite suffers from low capacity value (372 mA h g^{-1}) since

every six carbon atom can host only one lithium ion by forming a LiC_6 stoichiometry which is not suitable for the development of high energy density LIBs. Thus, seeking alternative anode materials is highly required. In this context, it has been recognized that graphene and other 2D materials such as, transition metal dichalcogenides (*e.g.*, MoS_2 , WS_2), transition metal oxide (*e.g.*, MoO_3 , Co_3O_4) are the potential materials for future LIB anodes due to their superior lithium storage capability with respect to that of graphite.

Therefore, during the three years of my PhD activity, I mainly concentrated on the research of anode materials based on graphene and MoS_2 . For what concerns graphene, I focused on the production first, investigating the effect of flakes morphology on the lithium-ion storage capability. As for MoS_2 , I carried out the production of few layers MoS_2 flakes and studied their lithium storage capability as well as sought a way to improve their electrochemical performance with respect to that of bulk MoS_2 and graphite.

The idea of size selection of graphene is to sort graphene flakes, by layer numbers and lateral size, figuring out the influence of lateral size and thickness of the flakes on the electrochemical performance upon lithiation/de-lithiation. This strategy will provide useful guidelines for the practical exploitation of few- (FLG) and multi- (MLG) layer graphene as stand-alone anode materials in LIBs. To achieve this target, I have produced graphene ink by liquid phase exfoliation (LPE) of pristine graphite. Besides, the activity of MoS_2 -based LIBs was carried out in order to provide the idea about production of nano-sized MoS_2 flakes and to fully understand the role of MoS_2 flakes in their electrochemical activities so that I can find the ways to improve lithium ion storage capability of this material. To achieve this, I have synthesized MoS_2 inks by LPE of bulk MoS_2 , studying the electrochemical properties of the as-produced MoS_2 flakes by sedimentation-based separation. Taking advantage of the MoS_2 flakes via LPE and anode fabrication, I have successfully fabricated and optimized MoS_2/C anodes with stable and enhanced electrochemical performance with respect to pristine MoS_2 anode. This work will give the research community a promising opportunity to exploit other carbon composite of 2D materials, such as transition metal chalcogenides and transition metal oxides as anode electrodes to improve their electrochemical performances.

ACTIVITY REPORT

Research Activity

Research Period Abroad

Scientific Publications

1. H. Sun, A. E. Del Rio Castillo, S. Monaco, A. Capasso, **D. A. Dinh**, A. Ansaldo, M. Prato, V. Pellegrini, B. Scrosati, L. Manna and F. Bonaccorso, *Binder-free graphene-based anode for Li ion battery*, Journal of Materials Chemistry A, 4, 6886-6895 (2016).
2. H. Sun, A. Varzi, V. Pellegrini, **D. A. Dinh**, R. Raccichini, A. E. Del Rio-Castillo, M. Prato, M. Colombo, R. Cingolani, B. Scrosati, S. Passerini, and F. Bonaccorso, *How much does size really matter? Exploring the limits of graphene as Li ion battery anode material*, Solid State Communication, 251, 88-93 (2017).

3. H. Sun, D. Hanlon, **D. A. Dinh**, J. B. Boland, A. E. Del Rio Castillo, C. D. Giovanni, A. Ansaldo, V. Pellegrini, J. N. Coleman and F. Bonaccorso, *Carbon nanotubes-bridged molybdenum trioxide nanosheets as high performance anode for lithium ion batteries*, **in press** 2D Materials 2017.

4. A. E. Del Rio Castillo, H. Sun, **D. A. Dinh**, J. Buha, A. Ansaldo, A. Capasso, L. Manna, V. Pellegrini, and F. Bonaccorso, *Solution processed black phosphorus in low boiling point solvents as efficient anodes for Li-ion battery*, **submitted**.

5. **D. A. Dinh**, H. Sun, L. Najafi, A. E. Del Rio Castillo, A. Ansaldo, Z. Dang, C. D. Giovanni, V. Pellegrini, and F. Bonaccorso, *Facile synthesis of MoS₂-flakes/amorphous-carbon composite as anode for lithium-ion batteries*, **submitted**.

Communications at Conferences

Oral communications:

1. H. Sun, A. E. Del Rio Castillo, **D. A. Dinh**, V. Pellegrini, and F. Bonaccorso, *Binder-free graphene-based anode for Li ion battery*, GrapChina, October 28-30, 2015, Qingdao, China.

2. Sun, A. Varzi, V. Pellegrini, **D. A. Dinh**, R. Raccichini, A. E. Del Rio-Castillo, M. Prato, M. Colombo, R. Cingolani, B. Scrosati, S. Passerini, and F. Bonaccorso, *How much does size really matter? Exploring the limits of graphene as Li ion battery anode material*, EMRS Spring Meeting, May 22- 26, 2017, France

3. **D. A. Dinh**, H. Sun, L. Najafi, C. Di Giovanni, A. Esau Del Rio Castillo, A. Ansaldo, Z. Dang, V. Pellegrini and F. Bonaccorso, *Carbon coated MoS₂ flakes as anode for lithium-ion batteries*, International Nanotech & Nanoscience Conference, June 28-30, 2017, France

4. **D. A. Dinh**, H. Sun, L. Najafi, C. Di Giovanni, A. Esau Del Rio Castillo, A. Ansaldo, Z. Dang, V. Pellegrini and F. Bonaccorso, *Facile synthesis of MoS₂-flakes/amorphous-carbon composite as anode for lithium-ion batteries*, Applied Nanotechnology and Nanoscience International Conference 2017, October 18-20, 2017, Italy

Poster Communications:

1. **D. A. Dinh**, H. Sun, A. E. Del Rio-Castillo, S. Monaco, A. Capasso, A. Ansaldo, M. Prato, V. Pellegrini, B. Scrosati, L. Manna and F. Bonaccorso, *Binder-free graphene film via solvent exchange process as anode in Li-ion battery*, Graphene 2016, April 19-22, 2016, Genova, Italy.

2. H. Sun, A. Varzi, **D. A. Dinh**, R. Raccichini, A. E. Del Rio Castillo, R. Cingolani, V. Pellegrini, B. Scrosati, S. Passerini, and F. Bonaccorso, *Influence of graphene flakes morphology on the lithium ion storage capability*, Graphene 2016, April 19-22, 2016, Genova, Italy.

3. **D.A. Dinh**, H. Sun, L. Najafi, C. Di Giovanni, A. Esau Del Rio Castillo, A. Ansaldo, V. Pellegrini and F. Bonaccorso, *Binder-free anode based on carbon-coated MoS₂*, the Italian national conference on materials Science and Technology, December 12-16, 2016, Catania, Italy.

4. H. Sun, A. Varzi, **D. A. Dinh**, R. Raccichini, A. E. Del Rio Castillo, R. Cingolani, V. Pellegrini, B. Scrosati, S. Passerini, and F. Bonaccorso, *How much does size really matter? Exploring the limits of graphene as Li ion battery anode material*, Graphene 2017, March 28-31, 2017, Barcelona, Spain.

Conferences Attended

Courseware

Courses attended and passed (credits)

Courses Given by Teachers of the Unige and IIT:

- 1) "Opto-Electronic Properties of Semiconductor Quantum Dots"
Dr. Moreels I. (18th February and 3rd, 10th March, IIT) – 1 credit.
- 2) "Energy storage and catalysis"
Dr. Colombo M., Dr. Monaco S. (17th, 19th, 24th, 26th March 2015, IIT) – 1 credit
- 3) "Basics of Crystallography"
Prof. Manna L. (29th April and 5th, 12nd, 19th May, IIT) – 1 credit.
- 4) "X-rays based Characterization Techniques"
Dr. Prato M., Dr. Palazon F. (22nd, 28th May 3rd, 9th June, IIT) – 1 credit.
- 5) "Electron microscopy"
Dr. Brescia R., Dr. Marotta R. (16th, 19th, 25th June, IIT) – 1 credit.
- 6) "Science and Technology of two-dimensional crystals"
Dr. Bonaccorso F. (July 1st-July 25th, IIT)- 1 credit.
- 7) "Characterization of polymeric materials, mechanical characterization"
Dr. Ceseracciu L., Dr. Heredia-Guerrero J. (5th, 6th, 17th, 18th May 2015, IIT)-4 credits.
- 8) "Electric circuits for Electrochemistry"
Dr. Ansaldo A., Dr. Gendron D. (30th June -14th July 2015, IIT)-3 credits
- 9) "Raman spectroscopy"
Prof. Carnasciali M. (June-July 2015, DCCI, **Università di Genova**) - 3 credits.
- 10) "Electrical and Raman characterization techniques"
Dr. Roman Krahne (September 26th-October 15th 2015, IIT) - 1 credit.
- 11) "Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations"
Dr. Luca de Trizio (February 22nd – March 9th 2017, IIT) - 1 credit.

Total credits: 18

Courses Given by invited experts:

- 1) "Modern Materials for Energy Saving (Renewable Energy)", Prof. Peter Rogl., Institute of Physical Chemistry, University of Vienna, Austria (9th -10th June 2015, DCCI, Università di Genova) – 1 credit.
- 2) "Green Analytical Chemistry", Prof. Estrella Espada Bellio, Facultad de Ciencias / Faculty of Science Universidad de Cádiz, Spain (26th -27th May 2015, DCCI, Università di Genova) – 1 credit.
- 3) "Novel Materials for energy storage and conversation"
Prof. Thomas Fassler (11th May 2017, DCCI, Università di Genova) – 1 credit

Total credit: 3

National and International Schools or Workshops

SCCER Summer School: Energy Storage in Batteries Materials, Systems and Manufacturing, July 11-15, 2016, Moschberg, Switzerland – 2 credits

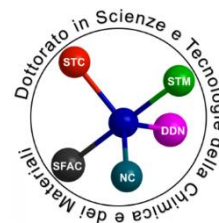
Total credit: 2

Other Activities



Università degli Studi di Genova

Doctorate in Sciences and Technologies of Chemistry and Materials



Curriculum: XXX

Mahdi Forouharshad

Start of the Doctorate Program *November 1st, 2014*

End of the Doctorate Program *November 1st, 2017*

Advisors

Prof. Orietta Monticelli

Thesis Title

Polymer nanoparticles and nanofibers: drug delivery and environmental applications

Thesis abstract

During the third year of my Ph.D., we focused on the preparation of poly(styrene-*co*-maleic anhydride) (PSMA) nanoparticles and on their use for an efficient conjugation with a model protein. Moreover, a preliminary work was performed on development and characterization of stereocomplex-poly(lactic acid) (sc-PLA) nanoparticles (NPs), prepared by nanoprecipitation and used as carrier of a drug model, namely 5,10,15,20-Tetrakis(4-hydroxy phenyl)-porphyrin (THPP). In this report, the results dealing with the former project will be summarized and a brief description of the work dealing with sc-PLA nanoparticles will be presented.

ACTIVITY REPORT

Research Activity

Research Period Abroad

During this 3rd year I was nine months at DTU University

1. Stereocomplex poly (lactic acid)/Porphyrin nanoparticles preparation and characterization
2. Silk fibroin/sc-PLA NPs/Porphyrin hydrogel preparation and characterization
3. Electrospun PLGA/sc-PLA NPs/Porphyrin preparation and characterization

Scientific Publications

1. Hyperbranched PDLA-polyglycerol: a novel additive for tuning PLLA electrospun fibers degradation and properties. Lorenza Gardella, Mahdi Forouharshad, Laura Pastorino, Orietta Monticelli, 2017, European Polymer Journal, 91: pp 21-30.
2. Bio-based System Composed of Electrospun sc-PLA/POSS/Cyclodextrin Fibers To Remove Water Pollutants, M. Forouharshad, M. Putti, A. Basso, M. Prato, O. Monticelli., 2015, ASC sustainable Chem. Eng., 3(11): pp 2917-2924.
3. A low-environmental-impact approach for novel biocomposites based on PLLA/PCL blends and high surface area graphite, M. Forouharshad, L. Gardella, D. Furfaro, M. Galimberti, O. Monticelli, 2015, European Polymer Journal, 70: pp 28–36.

Communications at Conferences

Poster Communications:

1. On a novel bio-system based on stereocomplex PLA for the removal of Pd catalysts, XXII national congress of the Italian of science and technology of macromolecules-AIM, Genova, Italy.

Congresses Attended

1. XXII national congress of the Italian of science and technology of macromolecules-AIM, Genova, Italy, 11-14 sep 2016.

Courseware

Courses attended and passed (credits)

Courses Given by Teachers of the Unige and IIT:

1. Nanoparticle characterization by atomic force microscopy and dynamic light scattering (2 credits)
2. Innovative pharmaceutical dosage forms: preparation and control methods (2 credits)
3. Pharmaceutical Biotechnology (3 credits)
4. Patent and bibliographic databases searching in medicinal chemistry (2 credits)
5. Polymeric nanocomposites (2 credits)
6. NMR spectroscopy(2 credits)

Courses Given by invited experts:

1. Yb and Eu strongly correlated electron systems: from experiment to interpretation of physical properties. Dott. Ivan Curlik (University of Presov, Slovachia), DCCI 22/04/2015.
2. Forensic chemical elements. Dott. R. Narizzano e F. Risso (ARPAL, Genova), DCCI, 19/05/2015.
3. Green Analytical Chemistry. Prof.ssa Estrella Espada Bellido (Dptm. of Analytical Chemistry, University of Cadiz, Spain), DCCI, 27/05/2015.
4. Modern Materials for Energy Saving (Renewable Energy). Prof. Peter Rogl (Institute of Physical Chemistry, University of Vienna, Austria), DCCI, 09/06/2015.
5. Conventional and Unconventional Superconductivity: An overview. Prof. Ernst BAUER (Institute of Solid State Physics, Vienna University of Technology, Austria), DCCI, 11/11/2015.
6. NIR spectroscopy: theory and applications, Dr. Tiziana Cattaneo and dr. Roberto Giangiacomo (CRA-IAA Council for Research in Agriculture and agrarian economy analysis) units research for jobs of agro-food industry engineering and food transformations, Milan) DIFAR, Genova, 29/02/2016.
7. Functional chromophores, syntheses and applications, Prof. Thomas J.J. (Heinrich Heine University, Dusseldorf), 9-10/06/2016, DCCI.
8. X-ray based experimental techniques and characterization of nano-materials. DCCI.

Seminars Attended

1. The bond between paper fibers: a fresh look at an old material. Prof. Robert Schennach (Inst. Solid State Physics, CD-Laboratory for Surface Chemical and Physical Fundamentals of Paper Strength, Graz University of Technology, Graz, Austria), DCCI, 17/02/2015.

2. Recent developments in the Processing of Ceramics and Glasses. Prof. Mike Reece (School of Engineering & Materials Science, Queen Mary University of London, UK), IENI-CNR Genova, 17/04/2015.
3. Design of magnetic nano-architecture. Dott. Davide Peddis (Istituto di Struttura della Materia, CNR – Roma), DCCI, 22/04/2016.
4. Diversity oriented synthesis of functional dyes – novel sequences, novel structures, novel properties. Prof. Thomas J.J. Müller (Heinrich Heine Universität, Düsseldorf), DCCI, 09/06/2016.
5. Metabolomics profile of hypoxic colorectal cancer cells. Dott. Alessandro Valli (Weatherall Inst. of Molecular Medicine, University of Oxford), DIFAR, 08/05/2015.
6. Hsp90 nella terapia antitumorale: dall'analisi conformazionale al disegno di nuovi inibitori allosterici. Dott. Gerolamo Vettoretti, DCCI, 25/05/2015.
7. Polymers and Composites from Renewable Resources. Prof. Alessandro Gandini (Institut Polytechnique de Grenoble, Universidade de São Paulo, São Carlo, Brazil), CNR, 23/09/2015.

National and International Schools or Workshops

1. XXXVII Congress-AIM School "Mario Farina" - Characterization of Polymeric Materials: Technical Polymer Cast and Solid State, Gargnano, Italy, 2-6 may 2016.



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



Curriculum: Chemical Sciences and Technologies

SOFIA-GAMBARO

Start of the Doctorate Program: November 1st, 2014

End of the Doctorate Program: October 31st, 2017

Advisors: M.L. Muolo (ICMATE-CNR) and Dr. Paola Riani (DCCI)

Thesis Title:

“Investigations of solid-liquid interactions in High Temperature Metal-Ceramic systems”

Thesis abstract

My PhD thesis is based on the investigation of solid-liquid interactions occurring in two different type of metal-ceramic systems (**oxidic** and **no oxidic**), representative of a **reactive** system in the first case and of a **reactive and dissolutive** system in the second one. To reach this goal a previous wettability evaluation of the systems in inert atmosphere is conducted. For both the systems the wetting test is performed using the sessile drop technique and the reactivity characterization using EDS analysis is evaluated: the sample sections are observed (LOM) and analysed (SEM-EDS).

The reactivity is investigated defining the different metal-ceramic phases formed at the interfacial zone. The interactions between the brazing alloys and the substrates have been also analysed by CALPHAD method; the experimental results are interpreted on the basis of thermodynamic calculations conducted using the thermodynamic databases. In the first case (oxidic system) an existing thermodynamic database is used [1] while in the second case (non oxidic system) a home-made (Al-C-Si-Ti) database is built merging the literature parameters and adapting them in order to obtain a self-consistent set of phase model and interaction parameters.

Reactive and **oxidic** system (YAG(Y₃Al₅O₁₂)/Ag-based alloy): after the wettability evaluation of YAG/pure metals and Ag-based alloys [2], a study of the joining samples (YAG/filler/Ti6Al4V) is conducted [3]. Different fillers (AgCuTi, AgCu, Ag) and temperatures have been taken into account. At the interfacial zone a thin and continuous metal-ceramic layer containing Ti is formed, in contact with the YAG, ensuring the adhesion between the joined materials.

The study of this metal-ceramic system is destined to obtain reliable joined materials to the sensor sector in the field of marine applications. The YAG is, indeed, characterized by an high level of transparency that is maintained also after the high temperature tests.

As a final step of the work, several samples representative of these materials are prepared and tested in terms of corrosion resistance in the marine water (ICMATE Bonassola laboratory); their evaluation is in progress.

Reactive/dissolutive not oxidic system (SiC/Al-Ti alloy): the wettability of SiC by two different Al-Ti alloys has been tested and the reactivity analysed changing process parameters, as temperature and time, and using the Differential Scanning Calorimetry, the EDS analysis and the CALPHAD

approach to understand the nature of the phases and predict the cooling path of the system (University of Lyon). The reactive and dissolutive SiC/filler alloy/SiC system is of great interest for the aerospace industry because the SiC shows an appealing combination of properties including high thermal, mechanical and chemical stability and low weight.

As a final step of the work, different joining samples have been produced changing the process parameters such as temperature and time and evaluated in terms of reactivity by the EDS analysis.

[1] O. Dezellus, R. Arroyave, S. Fries. Int J Res. 2011;v.102 (3), pp.286–97.

[2] S. Gambaro, M.L. Muolo, F. Valenza, G. Cacciamani, L. Esposito, A. Passerone. J.Eur.Ceram.Soc. 2015, v.35 (10), pp. 2895-2906.

[3] S. Gambaro, F. Valenza, A. Passerone, G. Cacciamani, M.L. Muolo, J.Eur.Ceram.Soc. 2016, v. 36 (16), pp. 4185-4196.

ACTIVITY REPORT

Research Activity

Research Period Abroad

From the 13th June to the 13th July 2016 and from the 30th October 2016 to the 30th March 2017 (6 months at Claude Bernard University of Lyon).

Scientific Publications

1. “Wettability of transparent YAG ($Y_3Al_5O_{12}$) by molten Ag–Cu–Ti alloys”
S. Gambaro, M.L. Muolo, F. Valenza, G. Cacciamani, L. Esposito, A. Passerone.
Journal of the European Ceramic Society, 2015, v.35 (10), pp. 2895-2906.
2. “Wetting study of the metal-ceramic system AgCuTi/YAG ($Y_3Al_5O_{12}$) for the production of YAG/AgCuTi/Ti6Al4V brazed joints”
S. Gambaro, F. Valenza, M.L. Muolo, A. Passerone, L. Esposito, J. Hostasa.
La Metallurgia Italiana, 2015, v.10, pp. 25-32.
3. “Brazing transparent YAG to Ti6Al4V: reactivity and characterization”
S. Gambaro, F. Valenza, A. Passerone, G. Cacciamani, M.L. Muolo.
Journal of the European Ceramic Society, 2016, v.36 (16), pp. 4185-4196.
4. “Wettability of SiC and graphite by Co-Ta alloys: evaluation of the reactivity supported by thermodynamic calculations”
S. Gambaro, F. Valenza, M.L. Muolo, A. Passerone, G. Cacciamani.
Journal of Materials Science, 2017, v.52 (23), pp. 13414–13426.
5. “Metal-ceramic interactions in brazing UHT diboride ceramics”
F. Valenza, C. Artini, **S. Gambaro**, M.L. Muolo, A. Passerone.
C. Artini ed. Alloys and Intermetallic Compounds: From Modeling to Engineering. Science publishers (an Imprint of CRC Press, Taylor and Francis Group), 2017.
6. “Surface engineering for joining SiC composites: effectiveness evaluated by surface analysis and wetting test”
F. Valenza, **S. Gambaro**, M.L. Muolo, A. Passerone, M. Salvo, V. Casalegno, M. Ferraris.
International Journal of Applied Ceramic Technology, 2017, v.14 (3), pp. 287-294.

7. "Wetting and interfacial phenomena of Ni-Ta alloys on CVD-SiC"
F. Valenza, **S. Gambaro**, M.L. Muolo, G. Cacciamani, P. Tatarko, T. Saunders, M.J. Reece, A. Schmidt, T. Schubert, T. Weißgärber, A. Passerone.
International Journal of Applied Ceramic Technology, 2017, v.14 (3), pp. 295-304.

Communications at Conferences

Oral communications:

1. Wetting study of the metal-ceramic system AgCuTi/YAG ($Y_3Al_5O_{12}$) for the production of YAG/AgCuTi/Ti6Al4V brazed joints"
S. Gambaro (sp), F. Valenza, M.L. Muolo, A. Passerone
AIM Conference (Associazione Italiana di Metallurgia); Rome (Italy) 5th-7th November, 2014.
2. "Investigation of Solid-Liquid Interactions in High Temperature Metal-Ceramic Systems"
S. Gambaro (sp), F. Valenza, M.L. Muolo, A. Passerone
29th Annual MSIT Meeting (International Seminar on Heterogeneous Multicomponent Equilibria) Schloss Ringberg, Tegernsee (Germany), 15th-20th February, 2015.
3. "Wetting and joining study of YAG/AgCuTi/Ti6Al4V system"
S. Gambaro (sp), F. Valenza, M.L. Muolo, L. Esposito, J. Hostasa, A. Passerone
High Temperature Capillarity Conference (HTC), Organized by Karlsruhe Institute for Technology (KIT)Bad-Herrenalb (Germany), 17th-21st May, 2015.
4. "Giunzioni metallo-ceramico (YAG-TiAlV): Studio della bagnabilità e della reattività mediante approccio termodinamico"
S. Gambaro (sp), F. Valenza, G. Cacciamani, M.L. Muolo, A. Passerone. Giornate di Istituto IENI-CNR, Padova, 29th February-1st March, 2016.
5. "Brazing transparent YAG to Ti6Al4V: wettability and reactivity characterization"
S. Gambaro (sp), F. Valenza, G. Cacciamani, M.L. Muolo, A. Passerone.
Journées Franco-Italiennes de Chemie (JFIC-2016), Avignon (France), 25th-26th April, 2016.
6. "Interfacial reactivity of the Al_3Ti -SiC system"
S. Gambaro (sp), F. Valenza, G. Cacciamani, M.L. Muolo, A. Passerone, O. Dezellus
EUROMAT (European Congress and Exhibition on Advanced Materials and Processes), Salonico, (Grecia); 17th-22th September, 2017.

Poster Communications:

1. "Wetting and reactivity of Ta-X (X=Ni, Co) alloys on CVD-SiC ceramics"
S. Gambaro, F. Valenza, A. Passerone, M.L. Muolo
High Temperature Capillarity Conference (HTC), Organized by Karlsruhe Institute for Technology (KIT); Bad-Herrenalb (Germany), 17th-21st May, 2015.
2. "Wetting and interfacial reactivity in the Ta-X (X = Co, Ni)/SiC system"
S. Gambaro, F. Valenza, A. Passerone, M.L. Muolo, G. Cacciamani
International Conference on Computer Coupling of Phase Diagrams and Thermochemistry (XLIV CALHAD); Loano (SV) Italy, 31 May-5 June 2015 (**Winner poster awards: 500\$**).
3. "Wetting and joining study of YAG/AgCuTi/Ti6Al4V systems"
S. Gambaro, F. Valenza, A. Passerone, M.L. Muolo, P. Riani
National School for PhD students in Inorganic Chemistry "New Materials and Sustainable Energy" (SCI-ENERCHEM); Bressanone (BZ) Italy, 13th-16th July, 2015.

4. "Wetting and reactivity in relation to SiC joining by Ta alloys"
S. Gambaro, F. Valenza, G. Cacciamani, M.L. Muolo, A. Passerone.
Giornate di Istituto IENI-CNR, Padova, 29th February-1st March, 2016.
5. "Surface engineering of SiC_i/SiC composites by *selective thermal removal*: effectiveness by surface analysis and wetting tests". F. Valenza, V. Casalegno, **S. Gambaro**, M.L. Muolo, A. Passerone, M. Salvo, M. Ferraris; Workshop Advanced manufacturing routes for metal/composites components for aerospace; Bruxelles (BE), 14th-15th September, 2016.
6. "Wettability of transparent YAG by molten AgCuTi alloys and joining study of YAG/AgCuTi/Ti6Al4V"
S. Gambaro, F. Valenza, A. Passerone, M.L. Muolo. Workshop DSCTM 2016 Sharing Knowledge and Expertise for a Better Society; Cetraro (Italy), 7th-9th September, 2016.
7. "Wetting and reactivity of Ta-X (X=Ni, Co) alloys on CVD-SiC ceramics"
F. Valenza, **S. Gambaro**, A. Passerone, M.L. Muolo. Workshop DSCTM 2016 Sharing Knowledge and Expertise for a Better Society; Cetraro (Italy), September, 2016.
8. "Wetting and interfacial reactivity in the Al₃Ti-SiC system"
S. Gambaro, F.Valenza, G.Cacciamani, M.L. Muolo, A. Passerone, F. Touche, R. Chiriac, O. Dezellus; XLVI CALPHAD; Saint-Malo, France, 11th-16th June, 2017.
9. "Wettability of transparent YAG by molten AgCuTi alloys and joining study of YAG/AgCuTi/Ti6Al4V"
S. Gambaro, F. Valenza, A. Passerone, G. Cacciamani, M.L. Muolo. EUROMAT (European Congress and Exhibition on Advanced Materials and Processes); Salonico, (Greece); 17th-22th September, 2017.

Other communications:

1. "Design of metal-ceramic interfaces for high temperature applications"
F. Valenza, **S. Gambaro**, A. Passerone, M.L. Muolo. European Symposium of Surface Science- 1st edition- Rome (Italy), 26th-28th November, 2014.
2. "The role of wettability in metal-ceramic systems in relation to joining of ceramic matrix composites"
F. Valenza, **S. Gambaro**, M.L. Muolo, A. Passerone. Workshop organized by TICASS consortium (Liguria Region); Genoa (Italy), 20th February, 2015.
3. "The role of surfaces and interfaces in liquid metal systems"
F. Valenza, S. Amore, **S. Gambaro**, D. Giuranno, , M.L. Muolo, R. Novakovic, A. Passerone, E. Ricci; XXII Conference AIV- Genoa (Italy), 20th-22th May, 2015.
4. "The role of the interfaces in metal-ceramic joints". A. Passerone, **S. Gambaro**, F. Valenza, M.L. Muolo. Queen Mary University and Nanoforce; London (UK), 16th June, 2015.
5. "Critical issue for producing brazed joints - wetting and reactivity"
A. Passerone, F. Valenza, **S. Gambaro**, M.L. Muolo. EUROMAT (European Congress of Advances Materials and Processes); Warsaw (Poland), 20th-24th September, 2015.
6. "Wetting of CVD-SiC by Ta alloys: the role of the testing procedure"
F. Valenza, **S. Gambaro**, M.L. Muolo, A. Passerone, T. Saunders, P. Tatarko, M. Reece EUROMAT (European Congress of Advances Materials and Processes); Warsaw (Poland), 20th-24th September, 2015.

7. "Wetting and reactivity of Ta-X (X=Ni, Co) alloys on CVD-SiC ceramics"
F. Valenza, **S. Gambaro**, A. Passerone, M.L. Muolo. Workshop DSCTM 2015 Sharing Knowledge and Expertise for a Better Society; Cetraro (Italy), 7th-9th October, 2015.
8. "Joining of SiC composites by Ta alloys: wetting studies and physical-chemical characterization of interfaces"
F. Valenza, **S. Gambaro**, M.L. Muolo, A. Passerone, M.J. Reece, T. Saunders, P. Tatarko, A. Schmidt, T. Schubert, T. Weissgaerber. AIDAA, Turin (Italy), 19th November, 2015.
9. "Wetting behavior and interfacial reactions in the Ir-Si/C system"
A. Camarano, D. Giuranno, **S. Gambaro**, R. Novakovic, E. Ricci, J. Narciso.
15th International Conference on High Temperature Materials Chemistry; Orleans (France), 29th March-1st April, 2016.
10. "Phase diagrams: a precious tool for the design of advanced brazing processes"
G. Cacciamani, F. Valenza, **S. Gambaro**, M.L. Muolo, A. Passerone. 36 Convegno AIM (Parma); 21st-23th September, 2016.
11. "Wetting and joining of SiC ceramics by Al-Ti alloys"; F. Valenza, **S. Gambaro**, M. L. Muolo, A. Passerone. EUROMAT (European Congress and Exhibition on Advanced Materials and Processes), Salonico, (Grecia); 17th-22th September, 2017.

Congresses Attended

1. **AIM** Conference (Associaz. Italiana di Metallurgia); Rome (Italy), 5th-7th November, 2014.
2. **MSIT 2015; International Seminar on Heterogeneous Multicomponent Equilibria**;
Schloss Ringberg, Tegernsee (Germany), 15th-20th February, 2015.
3. **HTC Conference** (High Temperature Capillarity Conference); Bad-Herrenalb (Germany), 17th-21st May, 2015.
4. **XLIV CALPHAD** Conference; Loano (Italy), 31th May-5th June, 2015.
5. **AIDAA 2015**; Oval Lingotto, Torino (Italy), 19th November, 2015.
6. **Journées Franco-Italiennes de la Chimie** (JFIC-2016), Avignon (France), 25th-26th April, 2016.
7. **Journées annuelles du GdR TherMatHt (Thermodynamiques des Matériaux et Hautes Températures)**, Limoges (France), 26th-27th January, 2017.
8. **XLVI CALPHAD** Conference; Saint-Malo, France, 11th-16th June, 2017.
9. **EUROMAT** (European Congress and Exhibition on Advanced Materials and Processes), Salonico, (Greece); 17th-22th September, 2017.

Courseware

During these 3 years Sofia Gambaro has acquired **12** credits of Courseware.

- Applicazione della spettroscopia RAMAN ai materiali (2 CFU, Prof. M.M. Carnasciali);
- Proprietà ottiche dei Materiali (3CFU, Prof. M. Canepa);
- Sintesi, struttura e proprietà funzionali di composti intermetallici (2CFU, Prof. A. Saccone);

- Fondamenti di microscopia elettronica a scansione ed in trasmissione (3CFU, Prof. P. Riani);
- Principi di metallurgia applicata: tradizione e innovazione (2CFU M.R. Pinasco).

Courses Given by Teachers of the Unige and IIT:

1. 03/03/2015 CNR-IENI, Genoa; *"Recent Cosmetic science and formulation technology"*; Prof. Yuji Yamashita (Pharmaceutical and Life Science Dept. - Chiba Institute of Science).
2. 17/04/2015, CNR-IENI, Genoa; *"Recent Developments in the Processing of Ceramics and Glasses"*; Prof. Mike Reece (Professor of functional ceramics School of Engineering & Materials Science; Queen Mary University of London (UK)).
3. 03/06/2015, CNR-IENI, Genoa; *"Pride and Prejudice on Oxygen"*; Prof. Joonho Lee (Korea, University, Seoul).
4. 22/09/2015, DCCI, Genoa: *"Electrochemical Impedance Spectroscopy – a tool for "in situ" investigation of SOFC anodes"*; Dott.ssa G. Raikova (Istituto di Elettrochimica e dei Sistemi Energetici (IEES) dell'Accademia Bulgara delle Scienze di Sofia).
5. 17/02/2015, DCCI, Genoa: IWIW 2016 International Workshop on Industrial Waste
6. 13/05/2016, CNR, Genoa, *"Carbon from a historical perspective"*; Javier Narciso Romero dell'Universidad de Alicante – Spain.
7. 27/05/2016, CNR, Genoa, *"SiC. Synthesis and Applications"*; Javier Narciso Romero dell'Universidad de Alicante – Spain.
8. 28/07/2016, CNR-CMATE, Genoa, *"Shear-Induced Release Model of Nano-Emulsion Prepared from Liquid Crystal"*; Prof. Yuji Yamashita; Department of Pharmaceutical and Life Science, Faculty of Pharmacy, Chiba Institute of Science, Japan.
9. 26/09/2016, CNR, Genoa, *"Biointerazioni dei reperti in ambiente marino"*; Dr. M. Faimali *CNR-ISMAR*.
10. 30/09/2016, IIT, Genoa *"Fragment-based drug discovery for identifying single- and multi-target inhibitors of CNS targets"*; Dr. Anders Bach, University of Copenhagen.
11. 20/10/2016, CNR, Genoa, *"Interazioni tra metalli liquidi e ceramici nei processi di colata di superleghe"*; Dr. Fabrizio Valenza, CNR-ICMATE of Genoa.
12. 06/03/2017, LMI University of Lyon 1 La Doua; *"2D Materials: the example of hexagonal boron nitride"*; Dr. Catherine Journet (IE CNRS, UCBL), Lyon (France).
13. 14/03/2017, LMI University of Lyon 1 La Doua; *" Thermal analysis techniques used for the characterization of materials"*; Rodica Chiriac (IE CNRS, UCBL), Lyon (France).
14. 11/04/2017, CNR Genova; *"Impatto dell'acqua sulle tecniche analitiche: HPLC, microbiologia, biologia molecolare"*; Marco Padovani, Field sales Specialist (SIGMA).
15. 20/04/2017, CNR Genova; *"Chemicophysical exchanges in TiC reinforced metal matrix composites"*; Dr. Olivier DEZELLUS; Université Claude Bernard Laboratoire des Multimatériaux et Interfaces (UMR 5615) Villeurbanne – Lyon, France.
16. 16/05/2017, DCCI Genova; *"Superfici ed interfacce in sistemi metallo-ceramici"*; Dr. A. Passerone; CNR-ICMATE Genova.
17. 26/06/2017, CNR Genova, *"Horizon 2020: come scrivere una proposta di successo"*; Dr.ssa N. Palazzo e Dr.ssa S. De Luca (CNR).
18. 29/09/2017, CNR Genova; *"Meta-analisi e replicabilità dei risultati"*; Prof. Massimiliano Pastore; Università di Padova.
19. 09/09/2017, CNR Genova; *"Materiali magnetocalorici"*; Corrado Tommasi; CNR-ICMATE sede di Lecco.

Courses Given by invited experts:

1. 31/03/15, DCCI, Genoa; “X-ray based experimental techniques and characterization of nano-materials”; Alberto Morgante (CNR-IOM and Physics Department Trieste University).
2. 21/04/2015 and 22/04/2015, DCCI, Genoa; “Yb and Eu Strongly Correlated Electron Systems: from Experiment to Interpretation of Physical Properties”; Dr. Ivan Curlik (University of Presov, Slovakia).
3. 09/06/2015 and 10/09/2015, DCCI, Genoa; “Modern Materials for Energy Saving (Renewable Energy)”; Prof. P. Rogl (Institute of Physical Chemistry, University of Vienna, Austria).
4. 23/06/2015, CNR-IENI, Genoa; “Polymers and Composites from Renewable Resources”. Prof. A. Gandini (Institut Polytechnique de Grenoble (Grenoble INP), FR); (5 hours of seminars followed).
5. 13/11/2015, DCCI, Genoa; “Medicinal chemistry with carbohydrates: the influenza virus and the discovery of sialidase inhibitors”; Prof. A. Bernardi (University of Milan).

National and International Schools or Workshops

1. **29th Annual MSIT Meeting:** International Seminar on Heterogeneous Multicomponent Equilibria; Schloss Ringberg, Tegernsee (Germany), 15th-20th February, 2015.
(Winner of Scholarship)
2. **National School** for PhD students in **Inorganic Chemistry** “New Materials and Sustainable Energy” (SCI-ENERCHEM); Bressanone (BZ) Italy, 13th-16th July, 2015.
(Winner of Scholarship GIFC)
3. **EMPA Workshop in Zurich-** Advanced Training Module: Shear Strength Testing of Joined Materials; EMPA (Swiss); 25th February, 2016.
4. **IWIW 2016 International Workshop on Industrial Waste;** DCCI Genoa (Italy), 17th February 2016.
5. **Workshop in Bruxelles (BE): Advanced manufacturing routes for metal/ composites components for aerospace;** 14th-15th September 2016.
6. **Journées annuelles du GdR TherMatHt (Thermodynamiques des Matériaux et Hautes Températures),** Limoges (France), 26-27 January, 2017.

Other Activities

1. Five days **group-work** on Fe-Zr phase diagram assessment at 29th Annual MSIT Meeting; Tegernsee (Germany); 13th-16th February, 2015.
2. “**Course of Security** in laboratories- ion radiation risk and radioprotection-“ (Dr. E. Ragno from CNR_Rome); Genova (Italy); 20th March, 2015.
3. **Two days Meeting and Results Discussion** with Project Officer of **European ADMACOM Project** (- FP7-F.o.F.-NMP-2013-10 GA609188 (ADvanced MANufacturing routes for metal/COMposite components for aerospace); Ottobrunn (Germany), 25th-27th March, 2015.

4. Ceremonial conference of **CNR-ISTEC** of Faenza (Italy) (main speakers: R. Brook, A. Tomsia, A. Bellosi), 28th April, 2015; “The new generation of ceramics” A. Tomsia (L. Berkeley National Lab., Ca, USA).
5. Six days **staff organizer** at XLIV CALHAD; Loano (SV) Italy, 31 May-5 June 2015.
6. Two days **Meeting** and **Results discussion** with Project Partners (Nanoforce); London (UK), 15th-17th June, 2015.
7. Two days **Meeting** and **Result discussion** with Project **Officer** of European ADMACOM Project (- FP7-F.o.F.-NMP-2013-10 GA609188 (ADvanced MANufacturing routes for metal/COMposite components for aerospace); Turin (Italy), 29th-30th September, 2015.
8. **Official member** in the **ADMACOM** European Project (European Commission DG Research & Innovation. *Key Enabling Technologies*; September 2015.
9. **Winner** of the **Short Term Mobility Program** for 21 days at LYON university (Ufficio Accordi e Relazioni Internazionali-CNR); 10th March, 2016.
10. **One day course of lab security** (Dr. M. Toselli; Dr. P. Santucci)-Corso di formazione:
 - **Rischio chimico e biologico in laboratorio**
 - **Gestione delle emergenze in laboratorio e nell’Area della Ricerca di Genova**CNR_IENI-Via de Marini 6 (Genoa); 21st March, 2016.
11. **Two weeks Co-tutor- Alternanza Scuola-lavoro- Studenti Liceo Giorgi.** CNR-Via de Marini 6 (Genoa); 9th-23th May, 2016.
12. **One day Meeting** and **Result discussion** with Project **POLITO Members** of European ADMACOM Project (-FP7-F.o.F.-NMP-2013-10 GA609188 (ADvanced MANufacturing routes for metal/COMposite components for aerospace); CNR-ICMATE, Genoa (Italy), 19th May, 2016.
13. **Three weeks** at Laboratoire des Multimaterieux et Interfaces- Université Claude Bernard de Lyon Domaine Scientifique de la DOUA; 43 Boulevard du 11 Novemnber 1918; **Thermodynamic evaluation of Al-C-Si-Ti system**; 13th June-3th July, 2016.
14. **One day Meeting** and **Results Discussion** with Project Officer of **European ADMACOM Project** (- FP7-F.o.F.-NMP-2013-10 GA609188 (ADvanced MANufacturing routes for metal/COMposite components for aerospace); Bruxelles (BE); 16th September 2016.
15. **Six months abroad** at **Laboratoire des Multimateriaux et Interfaces-** Université Claude Bernard de Lyon Domaine Scientifique de la DOUA; 43 Boulevard du 11 Novembre 1918; Lyon (France). **Thermodynamic evaluation of Al-C-Si-Ti system**; from 20 October 2016 to 31 of March. Supervisor: Prof. Olivier Dezellus.
16. **Certificated French Class for PhD student (36 hours).** Université Claude Bernard de Lyon Domaine Scientifique de la DOUA; 43 Boulevard du 11 Novembre 1918, Lyon (France).



Università degli Studi di Genova

Doctorate School in
Sciences and Technologies of
Chemistry and Materials

Curriculum: Nanochemistry

PhD candidate: Muhammad Imran

Start of the Doctorate Program *November 1st, 2014*

End of the Doctorate Program *October 31st, 2017*

Third year (01/11/2016 – 31/10/2017): Acyl Halides as a New Promising Precursors for the Colloidal Synthesis of Lead Halide Perovskite Nanocrystals

Tutors: Prof. Liberato Manna,

Cotutors: Prof. Maurizio Ferretti (Unige) & Dr. Luca Di Trizio (IIT)

Thesis abstract

Lead halide perovskite with the generic formula of $APbX_3$ [$A = Cs^+$ (Cesium), $CH_3NH_3^+$ (methylammonium, MA^+), $CH(NH_2)_2^+$ (formamidinium, FA^+); $X = Cl^-, Br^-, I^-$] have been intensively investigated both in the form of thin film and colloidal nanocrystals for various application owing to their excellent charge transport properties, high absorption coefficient, compositional tenability, low fabrication cost and most strikingly “defect-tolerance”. For instance within few years Perovskite solar cells have reached a certified power conversion efficiency of 22%, while the photoluminescence quantum yield (PL QY) of colloidally synthesized NCs is approaching unity (100%). Considering the limitation of the already proposed synthesis procedures we have devolved a simple single step synthesis approach for colloidal synthesis of lead halide perovskite nanocrystals by using acyl halide as a new promising halide precursor. This simple synthesis

method yield phase pure strongly fluorescent high quality nanocrystals of APbX₃ [A = Cs⁺ (Cesium), CH₃NH₃⁺ (methylammonium, MA⁺), CH(NH₂)₂⁺ (formamidinium, FA⁺); X = Cl⁻, Br⁻, I⁻]. The ease of adjusting the metal cations, anions, ligands and the adjustable injection temperature would open up a new avenue for the development of several stoichiometric and non-stoichiometric phases.

ACTIVITY REPORT

Research Activity

The research activity was mainly carried out at the IIT facilities in via Morego, 30 - Genova.

Scientific Publications

Original publications on ISI Journals:

1. **Imran M**, Di Stasio F, Dang Z, Canale C, Khan AH, Shamsi J, Brescia R, Prato M, Manna L. Colloidal synthesis of strongly fluorescent CsPbBr₃ nanowires with width tunable down to the quantum confinement regime. *Chemistry of Materials*. 2016, 28(18),6450-4.
2. Di Stasio F, **Imran M**, Akkerman QA, Prato M, Manna L, Krahne R. Reversible Concentration Dependent Photoluminescence Quenching and Change of Emission Color in CsPbBr₃ Nanowires and Nanoplatelets. *J. Phys. Chem. Lett.*, 2017, 8 (12), 2725–2729.
3. Dang Z, Shamsi J, Palazon F, **Imran M**, Akkerman QA, Park S, Bertoni G, Prato M, Brescia R, Manna L. In Situ Transmission Electron Microscopy Study of Electron Beam-Induced Transformations in Colloidal Cesium Lead Halide Perovskite Nanocrystals. *ACS Nano*, 2017, 11 (2), 2124–2.
4. Dang Z, Shamsi J, Akkerman QA, **Imran M**, Bertoni G, Brescia R, Manna L. Low-Temperature Electron Beam-Induced Transformations of Cesium Lead Halide Perovskite Nanocrystals. *ACS Omega*. 2017, 2(9), 5660-5.
5. **Imran M**, et.al. Acyl Halides as New Promising Precursors for the Colloidal Synthesis of lead halide Perovskite. (Preparation)
6. Caligiuri V, Milan P, **Imran M**, Manna L, Krahne R. Double-Epsilon-Near-Zero Cavities for Spontaneous Emission and Purcell Effect Enhancement. (Submitted)

Communications at Conferences

Poster Communications:

- 1) 2016, Lisbon, Portugal. 2nd International Symposium on Nanoparticles/Nanomaterials and Applications.
“Novel metal semiconductor heterojunction system obtained via thermal annealing of Cu₂S elongated nanocrystals”.
- 2) 2016, Genova, Italy. 2nd International Conference on Perovskite Solar Cells and Optoelectronics. “Colloidal synthesis of highly luminescent CsPbBr₃ nanowires with tuneable diameter down to the quantum-confined regime”

Courseware

Courses attended and passed

- 1) “Opto-Electronic Properties of Semiconductor Quantum Dots”
Dr. Moreels I. (18, 24 February and 3, 10 March, IIT) – 1 credit.
- 2) “Energy storage and catalysis”
Dr. Colombo M., dr. Monaco S. (17, 19, 24, 26 March 2015, IIT) – 1 credit
- 3) “Basics of Crystallography”
Prof. Manna L. (29 April and 5, 12, 19 May, IIT) – 1 credit.
- 4) “X-rays based Characterization Techniques”
Dr. Prato M., Dr. Palazon F. (22, 28 May 3, 9 June, IIT) – 1 credit.
- 5) “Electron microscopy”
Dr. Brescia R., Dr. Marotta R. (16, 19, 25 June, IIT) – 1 credit.
- 6) Science and Technology of two-dimensional crystals
Francesco Bonaccorso. (30 June and 7, 13, 20 July, IIT) – 1 credit.
- 7) “Magnetic properties and characterization techniques”
Dr. Lak A. (6-9-16 October, IIT) – 1 credit.
- 8) “Electrical and Raman characterization techniques”
Dr. Krahne R. (17-22-24 September, IIT) – 1 credit.
- 9) “Electronic properties of solids”

Prof. Manna L. (2-9-16-23 March, 1-13-20-27 April, 4-11-16 May, IIT) – 3 credits (corsi tipo B)

10) “Magnetic hyperthermia: from fundamental to biomedical applications”

Dr. Teran F. (5-6 May, 2016, IIT) – 1 credits (corsi tipo A)

11) “Laser-matter interactions: from fundamentals to applications” (3 credits) Dr. Marti Duocastella from 04/07/2017 to 25/07/2017

National and International Schools or Workshops

- 1) “DPG – School on Physics. Physical properties of nanoparticles: Characterization and applications”, 26-31 July 2015 Bad Honnef (Germany) – 4 credits.

Seminars Attended

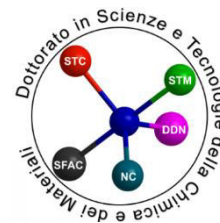
- 1) Dr. Francesco Di Stasio, “Semiconductor nanocrystals laser nanostructures”, IIT, 16/12/2016
- 2) Dr. Sedat Dogan, “Field effect transistor and solar cell made of individual colloidal PbS nanosheets”, IIT, 08/1/2015
- 3) Dr. Valeria Lotito, “Design, fabrication and characterization of plasmonic structures for graphene-based devices and superresolution”, IIT, 19/1/2015
- 4) Dr. Marco Agostini, “High Energy Lithium-Ion and Lithium-Sulfur Batteries”, IIT, 20/02/2015
- 5) Dr. Miri Kazes, “Using colloidal quantum dots to boost photocell performance”, IIT, 25/02/2015
- 6) Dr. J.C. Arnault, “Control of surface chemistry of nanodiamonds for bio-applications” IIT, 09/11/2015
- 7) Dr. Laura Miranda Perez, “Perovskites: an old materials for the third generation of PV solar panels” IIT, 21/04/2016

- 8) Dr. Giovanni Maria Vanacore, "Spatio-temporal visualization of atomic motions in low-dimensional materials" IIT, 03/05/2016.
- 9) Dr. Gwan-Hyoung Lee "Van der Waals Assembly of 2D materials for device applications" 16/01/2017
- 10) Stefano Amoroso "Theatrocracy: the communication in the modern age. IIT, 02/03/2017
- 11) Prof. Dmitri Talapin. "Synthetic methodology for colloidal nanomaterials: limitations and opportunities. IIT 26/05/2017.
- 12) Dr. Emory Chan High-throughput design of doped colloidal nanocrystals. IIT, 01/06/2017.
- 13) Prof. Bianxiao CUI "The Role of membrane curvature at the Nano-Bio interface". IIT, 12/09/2017
- 14) Helena Gavilan Rubio "Standardization methods for the synthesis of single-core and multi-core magnetic nanoparticles for medical applications". IIT 02/10/2017.
- 15) Dr. Ondrej L. Krivanek "Electron Microscopy Facility Seminar: "Aberration-corrected STEM: sub-Å resolution imaging, atomic-resolution elemental mapping, and vibrational spectroscopy" IIT, 04/10/2017.

Other Activities

Seminars Given

- 1) 07.01.2016, iit, NACH group meeting; "Novel metal semiconductor heterojunction system obtained via thermal annealing of Cu₂S elongated nanocrystals "
- 2) 21.04.2016, iit, NACH group meeting; "CsPbBr₃ Perovskite Nanowires"



Università degli Studi di Genova

Doctorate School in Sciences and Technologies of Chemistry and Materials

Curriculum: Nanochemistry

Viviana Maffeis

Start of the Doctorate Program November 1st, 2014

End of the Doctorate Program October 31st, 2017

Advisors

Prof. Renata Riva (UniGe) and Prof. Silvia Giordani (iit)

Thesis Title

“Functionalization of carbon nanomaterials for biomedical applications”

Thesis abstract

Carbon based nanomaterials are under intensive investigation as substrates for biomedical applications. The modification of nanomaterials with biologically active substrates such as glycopeptides, glycoproteins and antibodies offers a fascinating platform technology for developing targeted nanotherapeutics and vaccine candidates. With the emergence of biopharmaceuticals and immunotherapies at the forefront of modern medicine, there is a particular interest in the controlled chemical derivatization of carbon nanomaterials with biomolecules. Here, we describe an efficient strategy for the preparation of covalently modified carbon nano-onions (CNOs) using maleimido-sulphydryl ligation. The ligation methodology was applied to the preparation of both fluorescently labelled glycopeptide and fluorescently labelled protein conjugated CNOs. Localization and cell-viability studies demonstrated good biocompatibility and efficient cell-uptake of the modified CNOs. This finding has important implications for the future rational design of carbon nanomaterial based therapeutics. Soluble antigens, independent of some larger delivery vector, suffer from reduced uptake by APCs and poor immunogenicity. These fundamental flaws have led to the development of particle-based vaccine carriers that can more closely mimic the physiochemical characteristics of natural pathogens, enhancing antigen delivery to the immune system. Recently, nanotechnology has been applied to address the clear biomimicry challenge inherent to the next generation of more potent and sophisticated adjuvants. Although early adjuvants, such as aluminum hydroxide, have been successful in stimulating the immune response, the advent of nanoscale antigen delivery platforms has catalyzed the transition from these simple immunoactive chemical agents to adjuvants that can engage and direct immune responses more akin to the methods employed by pathogens themselves. Furthermore, I describe also a tunable application of a diiodo-BODIPY based photosensitizer. The CNO functionalization with the photosensitizer is achieved by π - π -stacking through a pyrene-anchoring group. The pyrene-diiodo-BODIPY derivative reveals an increase of the ROS basal level of HeLa cells, resulting in a remarkable photo-mediated cytotoxicity. Conversely, when the pyrene-diiodo-BODIPY / CNO nanohybrid is internalized by HeLa cells, no significant cytotoxicity is detected both with and without illumination. Just when the nanohybrids is disrupted and the

diiodo-BODIPY photosensitizer detaches from the CNO surface, a significant photo-induced cytotoxicity is observed. These results give important hints for the possible application of pyrene-diiodo-BODIPY-carbon nanomaterials nanohybrid based systems in photodynamic therapy.

ACTIVITY REPORT

Research Activity

The research activity was mainly carried out at the IIT. In 2015, I had the opportunity to work during the summer in the Organic Nano-materials research labs at University of Texas at El Paso. I was involved in the functionalization of cluster endohedral fullerenes, especially in the synthesis of *bis*-adducts of $M_3N@I_h-C_{80}$ ($M = Sc, Lu, Y, Er$), and the understanding of the factors controlling their regiochemistry using the independent (non-tethered) *bis*-1,3-dipolar cycloaddition reaction. In 2016 and 2017, I had the opportunity to spend 9 months at the School of Chemistry and Trinity Biomedical Sciences Institute, Trinity College Dublin working on the synthesis of fully synthetic glycopeptides.

International Internship

Date: 24/05/2015 – 02/08/2015

Visiting Research Student

University of Texas at El Paso, Department of Chemistry, El Paso, TX, USA

Research Project: 1,3-dipolar Cycloadditions on Endohedral Fullerenes $M_3N@I_h-C_{80}$ ($M=Sc, Lu, Y, Er$):

Remarkable Regiochemical Control by the Cluster

Supervisor: – **Prof. Luis Echegoyen**

Date: 07/03/2016 – 06/06/2016

Visiting Research Student

School of Chemistry and Trinity Biomedical Sciences Institute, Trinity College Dublin, Ireland

Research Project: Synthesis and Development of specific glycopeptides to translate complicated designs that work *in vitro* into a successful *in vivo* application

Supervisor: – **Prof. Eoin Scanlan**

Date: 01/04/2017 – 31/10/2017

Visiting Research Student

School of Chemistry and Trinity Biomedical Sciences Institute, Trinity College Dublin, Ireland

Research Project: Carbon nano-materials as photocatalysts in visible-light mediated, thiol-ene reactions

Supervisor: – **Prof. Eoin Scanlan**

Scientific Publications

Original publications on ISI Journals:

Frasconi, M.; Maffei, V.; Bartelmeß, J.; Echegoyen, L.; Giordani, S. *Methods Appl. Fluoresc.* 2015, 3 (4), 44005. Highly surface functionalized carbon nano-onions for bright light bioimaging

Cerón, M. R.; Maffei, V.; Stevenson, S.; Echegoyen, L. *Inorganica Chim. Acta* 2017. Endohedral fullerenes: Synthesis, isolation, mono- and bis-functionalization

Maffei, V.; Barnes, D.D.; Scanlan, M.E.; Giordani, S. Submitted. Efficient Covalent Immobilization of Glycopeptides and Proteins onto Carbon Nano-onions (CNOs)

Bartelmeß, J.; Maffei, V.; Signorelli, A., Giordani, S. In preparation. Unprecedented inhibited phototoxicity of a carbon nano-onion immobilized diiodo-BODIPY photosensitizer

Communications at Conferences

1. **NanotecC15 Carbon Nanoscience and Nanotechnology**, Oxford, UK, 14-17 September 2015
2. **NanotechItaly 2015**, Bologna, Italy, 24-27 November 2015
3. **Carbonhagen 2016 - 7th symposium on carbon and related nanomaterials**, Copenhagen, Denmark, 17-18 August 2016
4. **International Congress Engineering of Advanced Materials (ICEAM2017)**, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany, 10-12 October 2017

Courseware

During these 3 years Viviana Maffei has acquired **28.38 credits** of Courseware.

Courses attended and passed

- **General Courses: B-type Courses Given by Teachers of the iit: (9 credits)**

1) *Nanomaterials and Nanocomposites: Processing and characterization (7 hours)*

- Nanomaterials: Synthesis - methods and techniques I 28/01/2015
- Nanomaterials: Synthesis - methods and techniques II 03/02/2015
- Nanocomposites:
- Importance of composite and nanocomposite – Basic definitions
- Manufacturing methods – Mechanical properties 05/02/2015
- Composites of nanomaterials with polymers
- How nanocrystals behave in nanocomposite materials: Disordered Aggregations vs Self assembled structures

Speakers: Luca De Trizio; Milena Arciniegas, Vladimir Lesnyak

2) Opto-Electronic Properties of Semiconductor Quantum Dots (7 hours)

- Electrons in Free Space and Bulk Crystals 18/02/2015
- Band Structure of Bulk Metals, Insulators and Semiconductors 24/02/2015
- Confinement in 1, 2 and 3 Dimensions 03/03/2015
- Optical Properties of Semiconductor Quantum Dots 10/03/2015

Speaker: Iwan Moreels

3) Energy Storage and catalysis (7 hours)

- Introduction and fundamentals of heterogeneous catalysis 17/03/2015
- Catalysts characterization 19/03/2015
- Laboratory tests for gas-solid reactions 24/03/2015
- Basics on Li-ion batteries 26/03/2015

Speakers: Massimo Colombo, Simone Monaco

4) Characterization of functionalized and water soluble nanoparticles (9 hours)

- Inorganic nanoparticles for biological applications and their aqueous colloidal synthesis 10/04/2015
- Biomolecule functionalization of nanoparticles and characterization techniques for water soluble nanoparticles 14/04/2015
- Polymerization techniques at the nanoparticle surface 17/04/2015
- Characterization techniques for polymers 23/04/2015

Speakers: Teresa Pellegrino, Markus Barthel

5) Basics of Crystallography (7 hours)

- Symmetry, lattices and crystallographic systems 29/04/2015
- Space groups and overview of most common structures found in materials science 12/05/2015
- Crystallographic computing and the reciprocal lattice 19/05/2015
- Mathematical construction of a lattice

Speakers: Liberato Manna

6) Electrical and Raman characterization techniques (7 hours)

- Electrical properties of nanocrystals and nanocrystal films 17/09/2015
- Raman spectroscopy and lattice vibrations of nanocrystals 22/09/2015
- Applications in photo sensing and photovoltaics 24/09/2015

Speakers: Roman Krahne, Yang Zhang

7) Magnetic properties and characterization techniques (7 hours)

- Fundamentals of magnetism and magnetic properties of nanoparticles Part I 06/10/2015
- Fundamentals of magnetism and magnetic properties of nanoparticles Part II 09/10/2015
- Biomedical applications 16/10/2015

Speaker: Alberto Casu, Aidin Lak

8) Introductory course on transmission electron microscopy (7 hours)

- Introduction to transmission electron microscopy 10/06/2016
- Analytical electron microscopy 17/06/2016
- High-resolution TEM and in-situ TEM 21/06/2016
- Introduction to electron microscopy in biology, cryo (CryoEM) electron microscopy and electron tomography 30/06/2016

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

9) Science and technology of 2D crystals-(7 hours)

- Fundamentals: mechanical, optical and electrical properties 04/07/2016
- Production, processing and placement 12/07/2016
- Characterization 19/07/2016
- Applications 26/07/2016

Speaker: Francesco Bonaccorso

• **Advanced Courses: A-type courses Given by invited experts: (3 credits)**

- 1) X-ray based experimental techniques and characterization of nano-materials 31/03/2015**

Speakers: Alberto Morgante, CNR-IOM and Physics Department Trieste University

- 2) Medicinal chemistry with carbohydrates: the influenza virus and the discovery of sialidase inhibitors 13/11/2015**

Speakers: Anna Bernardi, Università di Milano

- 3) "NIR spectroscopy: theory and applications" 29/02/2015**

Speakers: Dr. Tiziana Cattaneo e Dr. Roberto Giangiacomo

National and International Schools or Workshops (6 credits)

1. **NMR DAY on Drug Discovery and Delivery: New Approaches**, Istituto Italiano di Tecnologia, Genova
16/10/2015
2. **Cancer Stem Cells and Autophagy: Diagnostic and Drug Discovery**, Istituto Italiano di Tecnologia, Genova
27/03/2017
3. **Micro and Nano Sensors: PhD summer school**, DTU Nanotech, Lyngby, Denmark, 14-25 August 2017

Seminars Attended: (3.38 credits)

- 1) **Design, fabrication and characterization of plasmonic structures for graphene – based devices and super – resolution**

Dr. Valeria Lotito 19/01/2015

- 2) **Designing organometallics for material science: application for solar cells and scintillators**

Dr. Guillaume Bertrand 19/01/2015

- 3) **Synergies between chemistry and nanotechnology: applications to neurosciences and energy**

Prof. Maurizio Prato 27/01/2015

- 4) **Colloidal Quantum Dot Optoelectronics: Photodetectors and Solar Cells**

Prof. Gerasimos Konstantatos 30/01/2015

- 5) **Printed Semiconductors and Novel 2-D Materials in the High Charge Density Regime**

Dr. Daniele Braga 04/02/2015

- 6) **Graphene towards real world applications: from epitaxy to supercapacitors**

Prof. Nunzio Motta 17/02/2015

- 7) **High Energy Lithium-Ion and Lithium-Sulfur Batteries**

Dr. Marco Agostini 20/02/2015

- 8) **Tetravalent DNA Nanostars as Valence-limited Building Blocks**

Dr. Lorenzo Rovigatti 02/03/2015

- 9) **Antral oocytes: chromatin organization and embryo development**

Drs. Manuela Monti nanophysics 03/11/2015

10) Control of surface chemistry of nanodiamonds for bio-applications	
<i>Dr. J.C. Arnault</i>	09/11/2015
11) Semiconductor Nanocrystals: Discovery, Milestones, and Recent Theoretical Developments	
<i>Prof. Alexander L. Efros</i>	20/11/2015
12) Synthesis and Chemical Manipulation of Nanoparticles for a Magnetic Improvement	
<i>Drs. Veronica Salgueirino</i>	11/12/2015
13) Natural polymers of bacterial origin and their medical applications	
<i>Prof.ssa Ipsita Roy</i>	18/12/2015
14) Recent advances with FIB-milled microcavities	
<i>Dr. Lucas Flatten</i>	19/01/2016
15) Materials for therapy: Cerium oxide nanoparticles as novel antioxidant drugs	
<i>Prof. Enrico Traversa</i>	04/02/2016
16) Ribosomes: a spectacular prebiotic machine	
<i>Prof. Ada Yonath</i>	15/02/2016
17) Functions and regulations of microRNAs in development and disease	
<i>Dr. Francesco Nicassio</i>	18/02/2016
18) Network of neurons and Carbon Nanotubes: interfacing neuronal growth and function	
<i>Prof. Laura Ballerini</i>	25/02/2016
19) Combined Light Harvesting and Charge Transfer in Complex Macromolecular Architectures	
<i>Prof. Amy M. Scott</i>	14/06/2016
20) Thermal forces: Moving and manipulating matter with thermal gradients	
<i>Prof. Roberto Piazza</i>	21/10/2016
21) From chemical complexity to functional complexity: tailoring multifunctional low dimensional materials and devices	
<i>Prof. Paolo Samorì</i>	14/11/2016
22) Van der Waals Assembly of 2D Materials for Device Applications	

<i>Prof. Gwan-Hyoung Lee</i>	16/01/2017
23) Photoactive systems for solar energy conversion, luminescence and catalysis	
<i>Prof. Nicola Armaroli</i>	27/01/2017
24) Colloidal double quantum dots	
<i>Dr. Dan Oron</i>	14/02/2017
25) Structural biopolymers – using Nature’s building blocks as an inspiration for advanced manufacturing	
<i>Dr. Benedetto Marelli</i>	01/03/2017
26) Interplay of electronic and dynamical processes in organohalide perovskites	
<i>Dr. Filippo De Angelis</i>	14/03/2017
27) The Future of Monitoring Serotonin (and Other Neurotransmitters) in Vivo	
<i>Dr. Anne M. Andrews</i>	20/03/2017

OtherActivities

Extra courses – VOLUNTARY **(3 credits)**

“Electronic properties of solids” held by Liberato Manna in iit

Class 1 - Crystals and Lattices

Class 2 - Basics of quantum mechanics

Class 3 - Hydrogen atom and orbitals

Class 4 - free electron theory

Class 5 - Quasi Free electron model I

Class 6 - Quasi Free electron model II

Class 7 - Tight Binding Theory for diatomic molecules and chains

Class 8 - Tight Binding for Linear Chains

Class 9 - Band Dynamics & quasi free electron in 2D lattices

Class 10 - 2D and 3D homopolar lattices, 2D heteropolar lattices

Class 11 -bands from p orbitals, bands from s and p orbitals

NACM talk: **(4 credits)**

TOT. credits: 28.38

Course certificate

Viviana Maffeis

Born 19 October 1990 has at the Technical University of Denmark passed the following PhD courses:

Year	ECTS points		7-grades-scale	ECTS scale
S17	5.0	Micro and Nano Sensors	PA	

The scale of marks used is:

- 7-grades-scale with the marks: -3 00 02 4 7 10 12
- PA/FA for passed/failed.

Kgs. Lyngby 20 September 2017



Tove Jensen
Office Assistant

List of Passed Subjects

Viviana Maffeis
Via Giardino 8
24029 Vertova (BG)
IT Italien

It is hereby confirmed that Viviana Maffeis, Civil Registration Number: 191090-VIM2, is enrolled as a student at Technical University of Denmark.

Name of the education: Gæst på Ph.d.-uddannelsen

The student graduated on 28.08.2017.

The student has passed the following subjects.

The credits are shown in ECTS-point

	Marks	ECTS- grade	Credits
Gæst på Ph.d.-uddannelsen	passed		5,0
Optional Courses in Ph.D-studies after 2002			5,0
Micro and Nano Sensors	PA		5,0



PhD Summer School

Micro- and Nano Sensors

Program 14-25 August 2017

Final Program

Week 1	Monday 14/8	Tuesday 15/8	Wednesday 16/8	Thursday 17/8	Friday 18/8	Saturday 19/8
8:30-9:00	Welcoming breakfast					
9:00-10:00	Practical issues <i>Anja Boisen</i>	Talk: "Abs, cells and organs on chip", <i>Albert van den Berg, University of Twente</i>	Talk: "Sensors in drug delivery" <i>Thomas Rodes, University of Copenhagen</i>	Talk: "Industrial perspective on formulation of vaccines" <i>Steffen Glismann, GlaxoSmithKline</i>	Lab group work	
10:00-11:00		Talk: "Optical sensors - an industrial perspective" <i>Tom Olesen, Biosense Solutions</i>	Talk: "Centrifugal microfluidics - an industrial perspective" <i>Robert Burger, BluSense</i>	Talk: "Global Challenges" <i>Jan Madsen, DTU Compute</i>		
11:00-12:00	10:30: Talk: "Introduction to sensors in drug delivery", <i>Anthony Turner, Linköping University.</i>	Talk: "Industry perspective", <i>Thomas S. Hansen, Radlometer</i>	Talk: "Resonators" <i>Peter Larsen, DTU Nanotech</i>	Talk: "Raman and SERS" <i>Tomas Rindzevicius, DTU Nanotech</i>		
12:00-13:00	Lunch Open space, Skylab	Lunch Open space, Skylab	Lunch Open space, Skylab	Lunch Auditorium, Skylab	Lunch Auditorium, Skylab	
13:00-14:00	Clean room safety course Bldg. 347, Danchip Seminar room	Planning/Lab group work	Lab group work	Lab group work	Lab group work	
14:00-15:00	14:30: Presentations from lab project responsible					
15:00-16:00	30 sec pitches about yourself and research					
16:00-17:00	Poster session with sodas, beers and snacks					
17:00-18:00					Social activity: Scenic boattrip around the canals in Copenhagen and dinner at Restaurant Påfuglen in Tivoli Gardens. Bus pick-up at 15:00, Ørsted's Plads in front of building 345C.	16:00 Optional social event
18:30	Welcoming dinner <i>Meyers Spisehus, Lyngby</i>					

Practical issues

Lectures

Social events

Group work

All activities take place in Bldg. 373A, Skylab auditorium unless otherwise stated.



PhD Summer School

Micro- and Nano Sensors

Program 14-25 August 2017

Final Program

Week 2	Monday 21/8	Tuesday 22/8	Wednesday 23/8	Thursday 24/8	Friday 25/8
9:00-10:00	Talk: "Life in academia and industry - the right steps to consider a successful career" <i>Thomas Rades, University of Copenhagen</i>	Lab group work	Lab group work	Poster and pitch preparation	Pitches (Evaluation panel: <i>Trine Wintenz, University of Copenhagen, Tom Olesen, BioSense Solutions, Ulrik Lytt Rahbek, Novo Nordisk</i>) Building 421, Auditorium 71
10:00-11:00	Talk: "Start-up perspective" <i>Trine Wintenz, University of Copenhagen, Filippo Bosco: BioSense, Gustav Skands: SBT Aqua</i>				
11:00-12:00	What to prepare for the pitch? <i>Anja Boisen</i>				
	11:10: Talk: "How to communicate science in a short pitch", <i>Andreas Møgelhøj, Haldor Topsøe</i>				
12:00-13:00	Lunch Open space, Skylab	Lunch Open space, Skylab	Lunch Open space, Skylab	Lunch Open space, Skylab	Lunch: BBQ Courtyard, DTU Nanotech
13:00-14:00	Lab group work	Lab group work	Lab group work	Poster and pitch preparation	Evaluation
14:00-15:00				14:00: Deadline for uploading the poster on campusnet	13:30: Poster session DTU Nanotech, Building 345C
15:00-16:00					
16:00-17:00					

Practical issues

Lectures

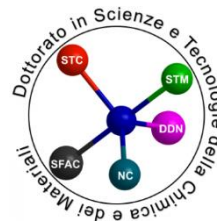
Social events

Group work

All activities take place in Bldg. 373A, Skylab auditorium unless otherwise stated.



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



Curriculum: Materials Science and Technology

GIOVANNI MANFREDI

Start of the Doctorate Program *November 1st, 2014*

End of the Doctorate Program *October 31st, 2017*

Advisors

Prof. Davide Comoretto

Thesis Title

Organic & Hybrid Photonic Crystals for Controlling Light-Matter Interaction Processes

Thesis abstract

Photonic crystals are systems obtained creating composite materials that present inside them a periodical distribution of media having different dielectric constant. Having reticular spacings with dimensions in the order of the wavelength of the visible spectrum, the interference patterns created by the photons diffracted crossing the dielectric lattice give rise to the formation of a photonic band structure that alter the behavior of the common light we see. In particular they operate a redistribution of the photonic density of states that changes the interaction between light and materials modifying the behavior of photoactive elements possibly included inside a photonic crystal. This thesis is focused on the study of the optical properties of materials inserted inside a photonic crystal that alters the common behavior of the electromagnetic field. In particular it will be discussed the use of this system for emission reshaping, lasing, and sensing.

ACTIVITY REPORT

Research Activity

Research Period Abroad

Dresden Integrated Center for Applied Physics and Photonic Materials (February 11th-November 1st 2016)

Scientific Publications

Original publications on ISI Journals:

- 1) **Lasing from Dot in-Rod Nanocrystals in Polymer Planar Microcavities**
Giovanni Manfredi, Paola Lova, Francesco Di Stasio, Prachi Rastogi, Roman Krahne, Davide Comoretto
ACS Photonics, **to submit**
- 2) **All-Polymer Photonic Microcavities Doped with Perylene Bisimide J-Aggregates**
Paola Lova, Vincenzo Grande, Giovanni Manfredi, Maddalena Patrini, Stefanie Herbst, Frank Würthner, Davide Comoretto
Advanced Optical Materials, DOI: 10.1002/adom.201700523
- 3) **Directional Fluorescence Spectral Narrowing in All-Polymer Microcavities Doped with CdSe/CdS Dot-in-Rod Nanocrystals**
Giovanni Manfredi, Paola Lova, Francesco Di Stasio, Roman Krahne, Davide Comoretto
ACS Photonics, 4, p. 1761 (2017)
- 4) **Cellulose ternary photonic crystal created by solution processing**
Giovanni Manfredi, Claudia Mayrhofer, Gerald Kothleitner, Robert Schennach, Davide Comoretto
Cellulose 23, p. 2853 (2016)

- 5) **In-plane anisotropic photoresponse in all-polymer planar microcavities**
Robert J. Knarr III, Giovanni Manfredi, Elisa Martinelli, Matteo Pannocchia, Diego Repetto, Carlo Mennucci, Ilaria Solano, Maurizio Canepa, Francesco Buatier de Mongeot, Giancarlo Galli, Davide Comoretto
Polymer **84**, p. 383 (2016)
- 6) **High Refractive Index Hyperbranched Polyvinylsulfides for planar one-dimensional all-polymer photonic crystals**
Serena Gazzo, Giovanni Manfredi, Robert Pötzsch, Qiang Wei, Marina Alloisio, Brigitte Voit, Davide Comoretto
Journal of Polymer Science PART B: Polymer Physics, **54**, p. 73 (2016)
- 7) **Polymer Distributed Bragg Reflectors for Vapor Sensing**
Paola Lova, Giovanni Manfredi, Luca Boarino, Antonio Comite, Michele Laus, Maddalena Patrini, Franco Marabelli, Cesare Soci, Davide Comoretto
ACS Photonics, **2**, p. 537 (2015)
- 8) **Hybrid ZnO:polystyrene nanocomposite for all-polymer photonic crystals**
Paola Lova, Giovanni Manfredi, Luca Boarino, Michele Laus, Giulia Urbinati, Tonia Losco, Franco Marabelli, Valentina Caratto, Maurizio Ferretti, Maila Castellano, Cesare Soci, Davide Comoretto
Physica Status Solidi (C), **12** p. 158 (2015)

Communications at Conferences

Oral communications:

- 1) **EMRS Fall meeting (Warsaw, September 17-21, 2017)**
Hybrid polymer inorganic microcavities using CdSe/CdS nanorods: from fluorescence enhancement to lasing
Giovanni Manfredi, Francesco Di Stasio, Roman Krahné, Davide Comoretto
- 2) **EOSAM 2016 (Berlin, September 26-30, 2016)**
Hybrid polymer inorganic microcavities using CdSe/CdS nanorods
Giovanni Manfredi, Francesco Di Stasio, Roman Krahné, Davide Comoretto
- 3) **EMRS 2015 (Lille, May 11-15, 2015)**
Polymer Photonic Crystal Vapor Sensors
Paola Lova, Maddalena Patrini, Franco Marabelli, Giovanni Manfredi, Antonio Comite, Michele Laus, Luca Boarino, Graziella Ianniello, Paola Rizzo, Christophe Daniel, Gaetano Guerra, Cesare Soci, Davide Comoretto
- 4) **ECOF 14 (Genova, June 29 – July 2, 2015)**
All-polymer flexible Distributed Bragg Reflectors and Microcavities
Giovanni Manfredi, Serena Gazzo, Robert J. Knarr III, Eliana Piccinini, Marina Alloisio, Davide Comoretto

Poster Communications:

- 1) **International School on Hybrid and Organic Photovoltaics ISOPHOS (Arbatax, September 3-7, 2017)**
Fluorescence enhancement and lasing from hybrid polymer inorganic microcavities containing CdSe/CdS nanorods
Giovanni Manfredi, Francesco Di Stasio, Roman Krahné, Davide Comoretto
- 2) **Macrogiovani 2017 (Trento, June 22-23, 2017)**
Polymer and Hybrid Materials for Photonic Crystals
Giovanni Manfredi, Paola Lova, Pavlo Perkhun, Alba Surace, Davide Comoretto
- 3) **EPF Summer School - Transport Phenomena in Polymers and Hybrid Materials (Gargnano, May 14-19, 2017)**
Polymer Photonic Crystals
Giovanni Manfredi, Alba Surace, Pavlo Perkhun, Paola Lova, Davide Comoretto
- 4) **XII CONVEGNO NAZIONALE DELL'ASSOCIAZIONE ITALIANA DI SCIENZA E TECNOLOGIA DELLE MACROMOLECOLE – AIM (Genova, September 11-14, 2016)**
Solution Processed Cellulose Ternary Photonic Crystal
Giovanni Manfredi, Claudia Mayrhofer, Gerald Kothleitner, Robert Schennach, Davide Comoretto
- 5) **XII CONVEGNO NAZIONALE DELL'ASSOCIAZIONE ITALIANA DI SCIENZA E TECNOLOGIA DELLE MACROMOLECOLE – AIM (Genova, September 11-14, 2016)**
Hybrid polymer inorganic microcavities using CdSe/CdS nanorods
Giovanni Manfredi, Francesco Di Stasio, Roman Krahné, Davide Comoretto
- 6) **20th European Symposium on Polymer Spectroscopy (Dresden, September 11-14, 2016)**
Polymer and hybrid photonic crystals
Giovanni Manfredi, Paola Lova, Chiara Bastianini, Paolo Giusto, Davide Comoretto
- 7) **ICES 15 (Messina, October 12-15, 2015)**
Hybrid polymer inorganic microcavities with CdSe/CdS nanocrystals
Giovanni Manfredi, Francesco di Stasio, Roman Krahné, Davide Comoretto

- 8) **15th European Polymer Federation Congress (Dresden, June 21 – 26, 2015)**
Vapor Sensing by All-polymer 1D Planar Photonic Crystals
 Paola Lova, Maddalena Patrini, Franco Marabelli, Giorgio Guizzetti, Giovanni Manfredi, Antonio Comite, Michele Laus, Luca Boarino, Graziella Ianniello, Paola Rizzo, Christophe Daniel, Gaetano Guerra, Cesare Soci, Davide Comoretto
- 9) **SPP 2015 (Santa Margherita Ligure, June 7-10, 2015)**
Plasmonic Nanostructures @ Photonic Crystals
 Davide Comoretto, Valentina Robbiano, Marco Cucini, Giovanni Manfredi, Eliana Piccinini, Marina Alloisio
- 10) **EMRS 2015 (Lille, May 11-15, 2015)**
Polymer Photonic Crystal Vapor Sensors
 Paola Lova, Maddalena Patrini, Franco Marabelli, Giovanni Manfredi, Antonio Comite, Michele Laus, Luca Boarino, Graziella Ianniello, Paola Rizzo, Christophe Daniel, Gaetano Guerra, Cesare Soci, Davide Comoretto
- 11) **Fourth International Symposium Frontiers in Polymer Science (Riva del Garda, May 20-22, 2015)**
Polymer Photonic Crystal Structures
 Emanuele Bozzoni, Simone Congiu, Serena Gazzo, Robert J. Knarr III, Filippo La Rosa, Giovanni Manfredi, Davide Comoretto, Paola Lova, Cesare Soci, Graziella Ianniello, Paola Rizzo, Christophe Daniel, Gaetano Guerra, Elisa Martinelli, Giancarlo Galli, Katia Sparnacci, Michele Laus, Luca Boarino, Massimiliano Lanzi, Giampaolo Zuccheri

Congresses Attended

1. EMRS Fall meeting (Warsaw, September 17-21, 2017)
2. Macrogiovani 2017 (Trento, June 22-23, 2017)
3. EOSAM 2016 (Berlin, September 26-30, 2016)
4. 20th European Symposium on Polymer Spectroscopy (Dresden, September 11-14, 2016)
5. ICES 15 (Messina, October 12-15, 2015)
6. ECOF 14 (Genova, June 29 – July 2, 2015)
7. SPP 2015 (Santa Margherita Ligure, June 7-10, 2015)
8. EMRS Spring Meeting 2015 (Lille, May 11-15, 2015)

Courseware

Courses attended and passed (credits)

Courses Given by Teachers of the Università di Pavia:

- 1) Fotonica (6 credits)

Courses Given by Teachers of the Unige and IIT:

- 1) Proprietà ottiche dei materiali (3 credits)
- 2) Analisi multivariata dei dati chimici (3 credits)

Courses Given by invited experts:

- 1) Elementi di Chimica Forense (1 credit)
- 2) Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials
 Novel Materials for energy storage and conversion

National and International Schools or Workshops

- 1) *International School on Hybrid and Organic Photovoltaics ISOPHOS (Arbatax, September 3-7, 2017)*
- 2) *EPF Summer School - Transport Phenomena in Polymers and Hybrid Materials (Gargnano, May 14-19, 2017)*
- 3) *Advanced Optical Materials and Devices International School (London, March 1-3, 2016)*

Other Activities

Seminars Attended

- 1) **Atomic structure and mass-production of size-selected nanoparticles (clusters)**
 Richard E. Palmer
 May 30, 2017, Genova

- 2) **All-Polymer Nano-Photonics: from Lasers to Sensors**
Davide Comoretto
March 29, 2017, Genova
- 3) **Electrical properties of chitosan-based composites: Towards active dielectrics for flexible electronics**
Lavinia Curecheriu
March 29, 2017, Genova
- 4) **3D Finite Element Method modelling of dielectric and ferroelectric properties of composite systems**
Leontin Padurariu
March 29, 2017, Genova
- 5) **Polymer-based Composites: Process-Structure-Properties Relationship**
Paola Stagnaro
March 29, 2017, Genova
- 6) **Synthesis of high permittivity nanoparticles by hydrothermal and solvothermal methods**
Vincenzo Buscaglia
March 29, 2017, Genova
- 7) **Dal problema astronomico alla strumentazione: essere a metà tra scienza e tecnologia**
Marco Landoni
February 3, 2017, Genova
- 8) **Fotopolimeri in astronomia: aspetti pratici e risultati in cielo**
Alessio Zanutta
February 3, 2017, Genova
- 9) **Sviluppo di nuovi materiali per olografia: dalla molecola al materiale**
Andrea Bianco
February 3, 2017, Genova
- 10) Nanoseminar cycle:
2D Crystals for Smart Life
Kaustav Banerjee
September 16, 2016, Dresden
- 11) Nanoseminar cycle:
Energy transfer and optical properties of light harvesting aggregates
Alexander Eisfeld
June 30, 2016, Dresden
- 12) NanoMod seminar cycle:
Pulse optimisation using Gaussian processes
Mehrdad Baghery
June 24, 2016, Dresden
- 13) Nanoseminar cycle:
Nanobiosensors-based diagnostics
Arben Merkoci
June 16, 2016, Dresden
- 14) **Information theory and thermodynamics: a way to formalize systems out of thermodynamic equilibrium**
Alessio Gagliardi
June 3, 2016, Dresden
- 15) **The bond between paper fibers: a fresh look at an old material**
Robert Schennach
February 17, 2015, Genova
- 16) **Le dimensioni contano: Metodi di sintesi di nanoparticelle organiche ed inorganiche**
Katia Sparnacci
May 28, 2015, Genova
- 17) **Polymers and Composites from Renewable Resources – Seminar series**
Alessandro Gandini
September 30, 2015, h 14-17
September 30, 2015, h 10-13
September 29, 2015, h 14-17
September 29, 2015, h 10-13
Genova



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



Curriculum: Nanochemistry

Mario Miscuglio

Start of the Doctorate Program *November 1st, 2014*

End of the Doctorate Program *October 31st, 2017*

Advisors

Prof. M. Canepa (UniGe), Prof. Roman Krahne (IIT)

Thesis Title

“Optoelectronics and plasmonics in graphene and related nano materials”

Thesis abstract

My research is mainly focused on graphene plasmonic and optoelectronic devices.

Due to its great features like relatively low loss, high confinement, excellent electrical properties, flexible feature and good tunability, graphene can be a promising plasmonic material alternative to the noble metals.

The aim of my work is to develop approaches for launching and conveying graphene plasmons towards efficient and reliable communication on a device scale.

At the same time, I am analysing, using numerical simulations, different designs of metal antennas and their coupling to graphene plasmons, as well as graphene based nanopatterned waveguides that can lead to a more efficient GP propagation.

In my third year, in collaboration with the Molecular Foundry at Lawrence Berkeley Lab, I also investigated the plasmon propagation in metal self similar antenna arrays both numerically and experimentally. A further step in the nanoscale light manipulation was taken by designing, fabricating and optically characterizing Spatial variant lattices employed as polarizers and lenses.

I was also actively involved in the fabrication, numerical analysis and experimental characterization of Gold and Graphene patterned Sierpinski Carpets.

Furthermore, In my second year I investigated the acoustic phonon modes in CdSe/CdS core-shell dot-in-rod by non-resonant Raman spectroscopy, comparing the experimental results with finite elements simulation, in order to have a better understanding of the localized nature of the acoustic vibration modes and their resonant frequencies.

Another project that I took part in, during the third year of my PhD was related to the characterisation of millimeter-sized Perovskite crystals, produced in our Laboratories, through conductive AFM measurement. Here my contribution was to obtain a better understanding of the macroscopic properties and photocurrent generation mechanisms of such crystals.

I was also recently involved in the fabrication and characterisation of Distributed FeedBack lasers (DFB), based on second order Bragg gratings, built with different periodicity, in order to coherently amplify the spontaneous emission of CdSe/CdS giant-shell nano crystals.

ACTIVITY REPORT

Research Activity

Scientific Publications

- 1) "Shape approaches for enhancing plasmon propagation in graphene" – M. Miscuglio, D. Spirito, Remo Proietti-Zaccaria, and R. Krahne (ACS Photonics)
- 2) "Confined Acoustic Phonons in Colloidal Nanorod Heterostructures Investigated by Non-resonant Raman Spectroscopy and Finite Elements Simulations" – Mario Miscuglio, Miaoling Lin, Francesco Di Stasio, Ping-Heng Tan, and Roman Krahne (Nano Letters)
- 3) Multiband Plasmonic Sierpinski Carpet Fractal Antenna – F. De Nicola, M. Miscuglio, N. Puthya, D. Spirito, M. Polini, R. Krahne, V. Pellegrini (Under Submission)

Projects

1. Accepted Standard proposal #4754, "*Light guiding and manipulation by plasmonic nanostructures*"- **Lawrence Berkeley National Laboratory**, (1 Cyclotron Road, Berkeley, 94720, United States)

Posters

- 1) **Graphene2016** "*Graphene Plasmon Propagation Enhancement through antennas and nanopatterning*" (Genova (Italy) - April 19-22, 2016)
- 2) N. S. P. Purayil, **M. Miscuglio**, F. De Nicola, D. Spirito, A. Tomadin, F. Tantussi, F. De Angelis, M. Polini, R. Krahne, V. Pellegrini "*Fabrication and characterization of plasmonic gold Sierpinski nanocarpet*" **Nanophotonics and Micro/Nano Optics International Conference 2017 (Barcellona)**, September 13-15, 2017, Barcelona, Spain. **2. M. Miscuglio**, Davide Spirito, Remo Proietti, Roman Krahne
- 3) "*Plasmons in nanostructured graphene*" **N2D 2017 (NanoPhotonics of 2d Materials)**, July 31- August 03, 2017, **San Sebastian**, Spain. **3. M. Miscuglio**, Davide Spirito, Remo Proietti, Roman Krahne
- 4) "*Shape Approaches for Enhancing Plasmon Propagation in Grapheme*" **Materials.it (Catania)**, December 12-17, 2016, Catania, Italia.

Talks

- 4) **Optoelectronics Group seminar** – Dec 4 – Sala Marconi
- 5) **Nach Group Seminar** – Jan 21 – Sala Montalcini
- 6) **Molecular Foundry 2016 User Meeting** "Shape Approaches for Enhancing Plasmon Propagation in Grapheme"
- 7) **Optoelectronics Group seminar** – June 10 – Sala Volta

Congresses Attended

- 1) Tutorial on Multi-scale simulation of two-dimensional materials based devices (by Gianluca Fiori and Giuseppe Iannaccone, University of Pisa, Italy)
- 2) Graphene2016 (Genova (Italy) - April 19-22, 2016)

- 3) Molecular Foundry 2016 User Meeting** (August 11, 2016 - August 12, 2016), **Lawrence Berkeley National Laboratory**, (1 Cyclotron Road, Berkeley, 94720, United States)

Courseware

During his first and second year of doctorate **Mario Miscuglio** has acquired 17 credits of Courseware.

Courses attended and passed (23 credits)

- A-type Courses: Courses Given by invited experts (2 **credits**):
 - 1) "Metabolomics Profile of Hypoxic Colorectal Cancer Cells", Research Scientist presso il Weatherall Institute of Molecular Medicine, University of Oxford, 8 maggio, Difar sezione Chimica del farmaco e del Prodotto cosmetico, Dott. Alessandro Valli
 - 2) "X-ray based experimental techniques and characterization of nano-materials" Alberto Morgante, CNR-IOM and Physics Department Trieste University), 31 marzo 2015 , h. 14,30 – 17,30 DCCI Aula 6

- B-type Courses Given by Teachers of the IIT (**21 credits**):
 - 1) "Applicazioni della spettroscopia Raman", Prof. Alberto Morgante, CNR-IOM and Physics Department Trieste University (31 March 2015, DCCI, Università di Genova) – 2 credits.
 - 2) "Laboratory of Optical Fluorescence Microscopy Methods" , Dr. Marta D'Amora – 3 credits.
 - 3) "Characterization of Polymeric Materials" Dr. J A. Heredia-Guerrero, Dr. L. Ceseracciu – 4 credits.
 - 4) "Opto-Electronic Properties of Semiconductor Quantum Dots"
Dr. Moreels I. (18, 24 February and 3, 10 March, IIT) – 1 credit.
 - 5) "Energy Storage and catalysis"
Massimo Colombo, Simone Monaco. (17, 19, 24, 26 March, IIT) – 1 credit.
 - 6) "Basics of Crystallography"
Prof. Manna L. (29 April and 5, 12, 19 May, IIT) – 1 credit.
 - 7) "X-rays based Characterization Techniques"
Dr. Prato M., Dr. Palazon F. (22, 28 May 3, 9 June, IIT) – 1 credit.
 - 8) "Electron microscopy"
Dr. Brescia R., Dr. Marotta R. (16, 19, 25 June, IIT) – 1 credit.
 - 9) "Science and technology of two-dimensional crystals"
Francesco Bonaccorso, (30/06 7, 13, 20 July) – 1 credit.
 - 10) "Electrical and Raman characterization techniques"
Roman Krahne – 1 CFU
 - 11) "Nano-plasmonic devices: from fabrication to applications"
Dr. Andrea Toma - 3CFU
 - 12) "Nanoparticle characterization by Atomic Force Microscopy and Dynamic Light Scattering"
R. Rolandi - 2 CFU

National and International Schools or Workshops

Research Abroad

- 1) **Nano-Optoelectronics – ICFO** – Mediterranean Technology Park, Av. Carl Friedrich Gauss, 3, 08860 Castelldefels (Barcelona), Barcelona, Spain
 - Date 18 Oct – 25 Oct
- 2) **Nanofabrication Facilities – Molecular Foundry** – 1 Cyclotron Road, Berkeley, 94720 United States
 - Date 26/07/2016 -30/09/2016
- 3) **Nanoimaging Facilities – Molecular Foundry** – 1 Cyclotron Road, Berkeley, 94720 United States
 - Date 26/04/2016 -02/06/2016

Seminars Attended (2.75 credits)

- 1) Mehdi H., “Plasmonic Nanomaterials”, IIT, 12/1/2015.
- 2) S. Passerini, , “Materials for sodium batteries” 16/01/15
- 3) Bertrand G., “Designing organometallics for material science: application for solar cells”, IIT, 19/1/2015.
- 4) Lotito V., “Design, fabrication and characterization of plasmonic structures for graphene-based devices and superresolution”, IIT, 19/1/2015.
- 5) M. Agostini, “Highly Energy Lithium-Ion and Lithium-Sulfur Batteries”
- 6) Kazes M., “Using colloidal quantum dots to boost photovoltaic cell performance”, IIT, 25/2/2015.
- 7) D. Braga, Printed Semiconductors and Novel 2D Materials in the High Charge Density Regime”
- 8) Konstantatos G., “Colloidal Quantum dot Optoelectronics: Photodetectors and solar cells”, IIT, 30/1/2015.
- 9) Freytag A., “Versatile fabrication of highly porous cryogels from noble metal nanoparticles”, IIT, 4/3/2015.
- 10) M. Colombo, “Structure-activity relationship in CO oxidation over bimetallic AuCu Nanocrystals: the role of nanocrystals size, composition and support interaction”
- 11) Kriegel I., “Plasmonic heavily doped semiconductor nanocrystals: from fundamentals to their nanoscale applications”, IIT, 26/11/2014.
- 12) Plasencia J. I. C., “Optics of CdSe/CdS nanocrystals: a theoretical overview”, IIT, 5/12/2014.
- 13) Motta N., “Graphene towards real world applications: from epitaxy to supercapacitors” IIT 17/02/2015
- 14) M. Sainato, Chemi-transistors gas sensors based on multicomponent nano materials
- 15) D. Basov, Nano Photonic Phenomena in Vander Waals Heterostructures, 8th June 2016
- 16) BAZZANO A., “Strumentazione di chimica analitica per l'esplorazione del sistema solare”
- 17) GARBARINO S., “The magic of diazomethane: advantages and drawbacks of an elusive reagent”
- 18) GARDELLA L., “Self-assembled block copolymers aggregates: application in drug delivery”
- 19) GHIARA G., “Introduzione alle pile a combustibile e ai fenomeni di degrado ad alta temperatura”
- 20) MARTINEZ ESPINOSA M. I., “Seeing Molecules: A Survey on Non-Optical Microscopies and their Applications”
- 21) SPALLAROSSA M., “The hydrogen autotransfer process”
- 22) TASSANO E., “Artificial Metalloenzymes: combining metal- and biocatalysis for organic synthesis”



Università degli Studi di Genova

Curriculum: Nanochemistry



Leyla Najafi

Start of the Doctorate Program November 1st, 2014

End of the Doctorate Program October 31st, 2017

Advisors: Dr Francesco Bonaccorso (IIT), Dr Vittorio Pellegrini (IIT), Dr Daniele Marrè (DIFI)

Thesis Title: Production and processing of graphene and 2D crystal-based inks for printable and flexible (opto)electronics

Thesis abstract

Graphene has recently gained attention as some of its properties are promising for electronics applications *e.g.*, high mobility, high conductivity, high transparency and so on. Additionally, excellent optical transmittance combined with its semi-metallic behavior makes it a valuable material for transparent contacts in fuel cells. However, as graphene is a material without any natural bandgap, it is deemed unfavorable for many applications (*e.g.*, transistors). Therefore, other 2D semiconducting materials are sought after. Molybdenum disulfide (MoS_2) and other transition metal dichalcogenides (TMDCs) offer real solutions in this area, as they are intrinsic semiconductors that can be exfoliated into 2D layers. In single-layer form, the absence of interlayer leads to optical and electronic properties that differ markedly from those of their bulk counterparts. For example, the electronic band structure transitions from an indirect gap (in bulk) to a direct gap in the monolayer form.

My Ph.D. research aims to synthesize 2D crystals, designing and producing high performance 2D crystals-based (opto)electronic devices. In the final stage, I also expanded my research by developing 2D crystal-based fuel cells platforms. In this context, the development of novel, sustainable methods for hydrogen production represents a significant research challenge. In fact, hydrogen, a critical chemical reagent and energy carrier, is currently produced from fossil fuels, which are limited in supply and create harmful CO_2 emissions when consumed. Photoelectrochemical (PEC) water splitting, a process in which H_2O is split into H_2 and O_2 using the energy from sunlight, is a promising technology for renewable hydrogen production. Efficient, inexpensive, stable, and scalable PEC water splitting materials and devices must be developed to make this process viable for widespread implementation. However, essential barriers such as the

creation of active catalysts, corrosion prevention strategies, and techniques for successfully integrating all required components of the device must be overcome.

I demonstrated a high yield liquid exfoliation method, in achieving high-quality 2D crystal nanoflakes. During my Ph.D., I deeply investigated the role of the hole selective layer (HSL) and catalyst by exploiting 2D crystals. I proved the successful HSL and catalyst capabilities of these 2D crystals for splitting water. I demonstrated that HSL is beneficial to improve the devices performance due to the optimization of charge carrier collection efficiency, thus, reducing charge carriers recombination effect. A target to be further investigated relies on the improvement of the long-term stability and efficiency of fuel cells by exploiting 2D crystals as charge carriers and efficient catalyst.

In summary, the research work in my Ph.D. aims to address the following objectives:

- (a) Synthesis and characterization of 2D flakes including graphene and TMDCs
- (b) Integration of such 2D flakes in optoelectronic and electrochemical devices.

Research Activity

The research activity was mainly carried out at the IIT premises.

Scientific Publications

1. Solution-processed graphene or SWCNTs/engineered MoSe₂ flakes heterostructures for efficient electrochemical hydrogen evolution reaction.

L. Najafi, S. Bellani, R. Oropesa-Nuñez, A. Ansaldo, A. E. Del Rio Castillo, M. Prato, and F. Bonaccorso. (submitted).

2. Non-noble 3d metal chloride-doped liquid phase exfoliated MoSe₂ nanoflakes for efficient, pH-universal electrochemical hydrogen evolution reaction.

L.Najafi, S. Bellani, R. Oropesa-Nuñez, A. Ansaldo, M. Prato, A. E. Del Rio Castillo and F. Bonaccorso. (submitted).

3. Conductive ITO nanoparticles break optical transparency/high-areal capacitance trade-off for advanced aqueous supercapacitors.

S. Bellani, L. Najafi, G. Tullii, A. Ansaldo, R. Oropesa-Nuñez, M. Prato, M.Colombo, M. R. Antognazza, F. Bonaccorso. (submitted).

4. Aging Effects in Interface-Engineered Perovskite Solar Cells with 2D Nanomaterials: a Depth Profile Analysis.

Y. Busby, A. Agresti, S. Pescetelli, A. Di Carlo, C. Noel, J.Pireaux, L. Najafi, S. Bellani, A. E. Del Rio Castillo, M. Prato, F.Bonaccorso, F. Fumagalli, and L. Houssiau. (submitted).

5. Ultra-long ambient stable and Scalable Perovskite Solar Cells using MoS₂ as hole transport interlayer.

G. Kakavelakis, I. Paradisanos, B. Paci, A. Generosi, M. Papachatzakis, T. Maksudov, A. E. Del Rio Castillo, L. Najafi, G. Kioseoglou, E. Stratakis, F. Bonaccorso, and E. Kymakis. (submitted).

6. Thioethyl-porphyrazine/Nanocarbon Hybrids for Photoinduced Electron Transfer.

S. Belviso, A. Capasso, E. Santoro, L. Najafi, F. Lelj, S. Superchi, D. Casarini, C. Villani, D. Spirito, S. Bellani, A. E. Del Rio Castillo, and F. Bonaccorso. (submitted).

7. Carbon coated MoS₂ flakes as anode for lithium-ion batteries.

D. A. Dinh, H. Sun, L. Najafi, A. E. Del Rio Castillo, A. Ansaldo, Z. Dang, C. Di Giovanni, V. Pellegrini, and F. Bonaccorso. (submitted).

8. Graphene and 2D materials for high efficient and stable perovskite solar cells.

A. Agresti, S. Pescetelli, L. Najafi, F. Bonaccorso, Y. Busby and A. Di Carlo, IEEE NANO 2017, 2017.(paper submission).

9. Solution-Processed Hybrid Graphene Flake/2H-MoS₂ Quantum Dot Heterostructures for Efficient Electrochemical Hydrogen Evolution.

L. Najafi, S. Bellani, B. Martin-Garcia, R. Oropesa-Nuñez, A. E. Del Rio Castillo, M. Prato, I. Moreels, and F. Bonaccorso, Chem. Mater. 29, 5782–5786 (2017).

10. Graphene-Based Hole-Selective Layers for High-Efficiency, Solution-Processed, Large-Area, Flexible, Hydrogen-Evolving Organic Photocathodes.

S. Bellani, L. Najafi, B. Martin-Garcia, A. Ansaldo, A. E. Del Rio Castillo, M. Prato, I. Moreels and F. Bonaccorso, J. Phys. Chem. C. 121, 21887–21903 (2017).

11. Few-layer MoS₂ flakes as a hole-selective layer for solution-processed hybrid organic hydrogen evolving Photocathodes.

S. Bellani, L. Najafi, A. Capasso, A.E. Del Rio Castillo, M. Rosa Antognazza and F. Bonaccorso, J. Mater. Chem. A, 5, 4384-4396 (2017).

12. Ruthenium Tetrazole Based Electroluminescent Device: Key Role of Counter Ions for Light Emission Properties.

H. Shahroosvand, L. Najafi, A. Sousaraei, E. Mohajerani, M. Janghour, and F. Bonaccorso, J. Phys. Chem. C, 120, 24965–24972 (2016).

13. Few-Layer MoS₂ Flakes as Active Buffer Layer for Stable Perovskite Solar Cells.

A. Capasso, F. Matteocci, L. Najafi, M. Prato, J. Buha, L. Cinà, V. Pellegrini, A. Di Carlo, F. Bonaccorso, Adv. Energy Mater, 6, 1600920 (2016).

14. Spray deposition of exfoliated MoS₂ flakes as hole transport layer in perovskite-based photovoltaics.

A. Capasso, A.E. Del Rio Castillo, L. Najafi, V. Pellegrini, F. Bonaccorso, F. Matteocci, L. Cinà, A. Di Carlo. IEEE NANO 2015.

Communications at Conferences

Invited talks

1. A. Agresti, S. Pescetelli, Y. Busby, F. Biccari, G Kakavelakis, L. Najafi, A. E. Del Rio Castillo, E. Kymakis, F. Bonaccorso, A. Vinattieri, and A. Di Carlo “*Graphene and perovskite: a winning combination for new generation photovoltaics*” Baltic Conference Series, 08 - 11 October 2017, Stockholm, Sweden.

Orals

1. D. A. Dinh, H. Sun, L. Najafi, A. E. Del Rio Castillo, A. Ansaldo, C. Di Giovanni, V. Pellegrini and F. Bonaccorso “*Facile synthesis of MoS₂-flakes/amorphous-carbon composite as anode for lithium-ion Batteries*” Applied Nanotechnology and Nanoscience International Conference 2017, 18-20 Oct. 2017, Rome, Italy.
2. D. A. Dinh, H. Sun, L. Najafi, C. Di Giovanni, A. E. Del Rio Castillo, A. Ansaldo, V. Pellegrini, and F. Bonaccorso, “*Carbon coated MoS₂ flakes as anode for lithium-ion batteries*” NanoMaterials for Energy and Environment, 28 - 30 June 2017, Paris, France.
3. S. Bellani, L. Najafi, B. Martín-García, A. Ansaldo, A. E. Del Rio Castillo, M. Prato, I. Moreels and F. Bonaccorso “*Graphene-based Hole Selective Layers for High-efficiency, Solution-processed, Large-area, Flexible, Stable Hydrogen-Evolving Organic Photocathodes*” Graphene 2017, 28-31 March 2017, Barcelona, Spain.
4. L. Najafi, S. Bellani, A. Capasso, A. E. Del Rio Castillo, M. R. Antognazza, and F. Bonaccorso, “*Few-layer MoS₂ Flakes as Hole-selective Layer for Solution-processed Hybrid Organic Hydrogen-evolving Photocathodes*” Graphene 2017, 28-31 March 2017, Barcelona, Spain.
5. A. Capasso, F. Matteocci, L. Najafi, V. Pellegrini, A. Di Carlo, F. Bonaccorso, “*Stable perovskite solar cells with a MoS₂ active buffer layer*” RPGR 2016, 25-29 September 2016, Seoul, Korea.
6. A. Capasso, F. Matteocci, L. Najafi, M. Prato, V. Pellegrini, A. Di Carlo, F. Bonaccorso, “*MoS₂ flakes as hole transport layer in perovskite-based photovoltaics*” Graphene Week 2016, June 13-17, 2016, Warsaw, Poland.

7. A. Capasso, F. Matteocci, L. Cinà, A.E. Del Rio Castillo, L. Najafi, V. Pellegrini, A. Di Carlo, F. Bonaccorso "Spray deposition of exfoliated MoS₂ flakes as hole transport layer in perovskite-based photovoltaics" IEEE Nano 2015, 27-30 July, Rome (Italy).

Posters

1. L. Najafi, A. Capasso, F. Matteocci, M. Prato, J. Buha, L. Cinà, V. Pellegrini, A. Di Carlo, F. Bonaccorso "Few-layer MoS₂ flakes as active buffer layer for stable perovskite solar cells." 2st International Conference on Perovskite Solar Cells and Optoelectronic. 26-28 September 2016, Genova, Italy.
2. L. Najafi, A. Capasso, A.E. Del Rio Castillo, V. Pellegrini, F. Bonaccorso, F. Matteocci, L. Cinà, A. Di Carlo. "Stable perovskite solar cells with spray deposition of exfoliated MoS₂ flakes as hole transport". XXth International Krutyn Summer School. 12-18 June 2016, Warsaw, Poland.
3. L. Najafi, A. Capasso, F. Matteocci, M. Prato, J. Buha, L. Cinà, V. Pellegrini, A. Di Carlo, F. Bonaccorso. "Exfoliated MoS₂ flakes as hole transport layer in perovskite-based photovoltaics." Graphene 2016. 19-22 April 2016, Genova, Italy. (Winner of student poster award)
4. S. Belviso, A. Capasso, E. Santoro, L. Najafi, F. Lelj, S. Superchi, D. Casarini, C. Villani, D. Spirito, S. Bellani, A. E. Del Rio Castillo, and F. Bonaccorso. "Supramolecular hybrids of thio-ethylporphyrazine with graphene and carbon nanotubes for photo induced electron transfer." Graphene 2016. 19-22 April 2016, Genova, Italy.
5. L. Najafi, A. Capasso, F. Matteocci, M. Prato, J. Buha, L. Cinà, V. Pellegrini, A. Di Carlo, F. Bonaccorso. "MoS₂ flakes as a hole transport material for stable perovskite solar cells." 1st International Conference on Perovskite Solar Cells and Optoelectronic. 27-29 September 2015, Lausanne, Switzerland.
6. L. Najafi, S. Belviso, A. Capasso, E. Santoro, F. Lelj, S. Superchi, D. Casarini, C. Villani, D. Spirito, S. Bellani, A. E. Del Rio Castillo, and F. Bonaccorso. "Hybrids of thio-ethylporphyrazine with nano carbons for photo induced electron transfer." International Conference on Hybrid and Organic Photovoltaics. 10-13 May 2015, Rome, Italy.

Courseware

Courses attended and passed: 30 Credits.

Course Title	Starting date	Credits	Speaker	Location
Novel Materials for energy storage and conversion	2017	1	Prof. Dr. Thomas Fässler	Genova university
Spectroscopies for chemical analysis	2016	1	Francisco Palazon, Roman Krahne, Sandeep Ghosh	IIT
Electrochemistry	2016	1	Simone Monaco Sebastiano Bellani Haiyan Sun	IIT
Opto-Electronic Properties of Semiconductor Quantum Dots	2015	1	Iwan Moreels	IIT
Energy Storage and catalysis	2015	1	Massimo Colombo, Simone Monaco	IIT
Characterization of functionalized and water soluble nanoparticles	2015	1	Teresa Pellegrino, Markus Barthel	IIT
Basics of Crystallography	2015	1	Liberato Manna	IIT
X-rays based Characterization Techniques	2015	1	Mirko Prato	IIT
Electron microscopy	2015	1	Rosaria Brescia, Roberto Marotta	IIT
Science and Technology of two-dimensional crystals	2015	1	Francesco Bonaccorso	IIT
Characterization of Polymeric Materials	2015	4	Luca Ceseracciu , José Alejandro Heredia-Guerrero.	IIT
Applicazione della spettroscopia RAMAN ai materiali	2015	2	Marilena Carnasciali	Genova university
Green Analytical Chemistry	2015	1	Estrella Espada Bellido	Genova university
Laboratory of Optical Fluorescence Microscopy Methods	2015	3	Marta d'Amora	IIT
Conventional and Unconventional Superconductivity: An overview	2015	1	Prof. Ernst Bauer	Genova university

Electric circuits for electrochemistry	2015	3	Alberto Ansaldo , David Gendron	IIT
Magnetic properties and characterization techniques	2015	1	Aidin Lak	IIT
SUMMER SCHOOL Advanced Perovskite, Hybrid and Thin-film Photovoltaics	2016	5	Dr Wolfgang Tress Prof. Emilio Palomares, Dr Karsten Walzer , Prof. Hari Upadhyaya, Prof. Stuart Irvine, Prof. Dave Worsley, Prof. Bryce Richards, Dr. Jake Bowers, Prof. Piers Barnes, Prof. Neil Robertson, Dr Michal Maciejczyk , Dr Olga Malinkiewicz,	International Krutyn Summer School 2016 Krutyn, Poland

Seminars Given

1- Title: Preparation of MoS₂ QD and discuss about photoluminescence of MoS₂ QD and application of that in battery.

By: Leyla Najafi

Date: 10 May 2016 14:00-16:00 at IIT

2- Title: Solution-processed 2D materials for energy conversion applications.

By: Leyla Najafi

Date: 13 October 2017 12:00-13:00 at university of Rome "Tor Vergata"

Workshop Attended

Fabrication perovskite solar cell. 2-13 October 2017, University of Rome "Tor Vergata"

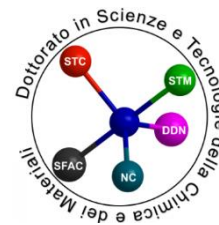
Seminars Attended

- 1) José A. Garrido, "CVD-based graphene field-effect transistor and electrodes", IIT, 10/12/2014.
- 2) Francesco Di Stasio, "Colloidal semiconductor nanocrystals laser structures", IIT, 16/12/2014.
- 3) Prof. Prato, "Synergies between chemistry and nanotechnology: applications to neurosciences and energy" IIT, 27/01/2014
- 4) Stefano Passerini, "Materials for sodium batteries", IIT 16/01/2015.
- 5) Valeria Lotito, "Design, fabrication and characterization of plasmonic structures for graphene-based devices and super-resolution", IIT, 19/1/2015.
- 6) Maurizio Prato, "Synergies between chemistry and nanotechnology: application to neurosciences and energy", IIT, 27/01/2015.
- 7) Gerasimos Konstantatos, "Colloidal Quantum dot Optoelectronics: Photodetectors and solar cells", IIT, 30/1/2015.
- 8) Franco Cacialli, "The power of intermolecular interactions in organic semiconductors : from threaded molecular wires to PCBM single crystals" IIT, 5 may 2016.
- 9) Csaba Janaky, "Hybrid nanoscale architectures of semiconductors and carbon nanomaterials- synthetic aspects and photoelectrochemical applications" IIT, 10 June 2016.
- 10) Alexander L. Efros, "Semiconductor nanocrystals: discovery, milestones, and recent theoretical development" IIT, 20 November 2015.

- 11) Dmitri N. Basov, "None-photonic phenomena in van der waals hetrostructures" IIT , 8 June 2016
- 12) Duc Anh Dinh, Lin Chen, "Introduction of basic electrochemical cell and lithium ion batteries" IIT, 23 June 2016.
- 13) Peter Reiss, " Insight in chemistry of metal sulfide nanocrystals and their application in photovoltaics" IIT, 25 November 2015.
- 14) Luigi Colombo, " Growth of Mono- and Bi-layer Graphene Single Crystals" IIT, 1 December 2015.
- 15) Filippo De Angelis, "Interplay of electronic and dynamical proless in organo halide perovskite" IIT, 14 March 2017.
- 16) Klaus Ensslin "Mesoscopic thermodynamics" IIT, 7 February 2017.
- 17) Slaven Garaj " Graphene based membranes" IIT, 11 April 2017.
- 18) Gwan Hyoung Lee "van der walls assembly of 2D materials for device applications" IIT, 16 January 2017.
- 19) Sameer Sapra "Perovskite nanocrystals- the new generation of defect tolerant luminescent materilas. IIT, 13 Jun 2017.
- 20) Francesca M. Toma" Intergrated photoelectrodes for CO₂ reduction and water oxidation " IIT, 13 Jun 2017.



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



Curriculum: SFAC

SARA PASTORINO

Start of the Doctorate Program: *November 1st, 2014*

End of the Doctorate Program: *October 31st, 2017*

Advisors: *Prof. Gabriele Caviglioli*

Thesis Title: *"Study of derivatives for diagnostic imaging of early atheromatous lesions"*

Thesis abstract

Atherosclerosis is a disease in which the intima of arteries thickens as a result of invasion and accumulation of white blood cell and remnants of dead cell, including cholesterol and triglycerides. Typically, atherosclerosis begins in childhood, as a thin layer of white-yellowish streaks in the artery walls and progresses to form a fibrofatty plaque. Atherosclerosis is asymptomatic for decades and even if the arteries enlarge at the plaque location, there is not immediately effect on blood flow. Symptoms occur after that the stenosis of artery is so severe (usually over 80%) than the blood supply to tissues is insufficient, and this induce the cardiovascular disorder such as stroke or heart attack.

My PhD project aims to develop a new system for the imaging of atherosclerotic lesion in an early stage of the disease, before the cardiovascular event.

Atheromatous plaques can be diagnosed by intravascularly administration of biologically active molecules with high affinity for some typical elements of the plaque and not present in the healthy artery walls. Then, these molecules must be conjugated with a system labeled with radionuclides γ -emitting or β^+ -emitters, detectable respectively through SPECT or PET or with magnetic agents detectable by MRI systems.

Different molecules have been studied, such as lipoproteins, peptides, oligopeptides, antibodies, carbohydrates, antisense nucleotides, and nanoparticles, but no system, for the moment, has entered in clinical practice. At the present, the biggest limitation is that this conjugate must quickly concentrate in the small volume of the plaque, in order to emit a signal significantly higher than the background, delivered by the free system in the blood. An ideal system combine high affinity and specificity for some elements of the lesion, with a good solubility and stability in vivo and in vitro, small dimensions and high blood clearance. In practice, the rate of incorporation of the conjugated system in the lesion should be significantly higher than the rate of elimination from the blood compartment. Furthermore, the rate of decay of the incorporated signal of radionuclides should be less than the rate of elimination of the system from the blood compartment.

DOTA (1,4,7,10-tetraazacyclododecane- N, N', N''N'''-tetraacetic acid) is a macrocyclic chelating agent, used in nuclear medicine for the ability to form stable complexes with metals.

Usually it is functionalized or its derivatives are used (such as para benzyl isothiocyanate, N-hydroxysuccinimide and maleimido-monoamide) in order to conjugate biologically active molecules.

These molecules must be specific and selective for the target of vascular lesion and do not compete, to focus in the plaque, with other molecules naturally present in the bloodstream.

VCAM-1 is a protein not detectable in the vessel tissue in physiological conditions, but is rapidly upregulated on vascular endothelium both in the initial and advanced lesion. In particular, VCAM-1 is the ligand for VLA-4, an integrin present on the surface of leukocytes. The binding between VCAM-1 and VLA-4 is possible if leukocytes are activated by chemotactic stimuli produced by damaged endothelial cells, which alter the conformation of the integrin VLA-4, giving high affinity binding to VCAM-1. Since the inflammatory process that leads to the development of a vulnerable atherosclerotic plaque is characterized by a high recall of monocytes and lymphocytes, which infiltrate the vascular wall at the point of the lesion, VCAM-1 is considered one of the most promising markers for imaging of vascular inflammation in atherosclerosis.

For this reason, the aim of my PhD project is to synthesize a molecule able to bind a ligand peptide specific and selective for VCAM-1 and to conjugate a chelating agent, such as DOTA or its derivatives, for the imaging.

ACTIVITY REPORT

Research Activity

Scientific Publications

- 1) "Development and characterization of a mucoadhesive sublingual formulation for pain control: extemporaneous oxycodone films in personalized therapy". Brunella Parodi, Eleonora Russo, Sara Baldassari, Guendalina Zuccari, Sara Pastorino, Mengying Yan, Karthik Neduri & Gabriele Caviglioli. *Drug Development and Industrial Pharmacy*, 43:6, 917-924.
- 2) "Development of an Injectable Slow-Release Metformin Formulation and Evaluation of Its Potential Antitumor Effects in a Pilot Study". Sara Baldassari, Agnese Solari, Guendalina Zuccari, Giuliana Drava, Sara Pastorino, Carmen Fucile, Valeria Marini, Antonio Daga, Alessandra Pattarozzi, Alessandra Ratto, Angelo Ferrari, Francesca Mattioli, Federica Barbieri, Gabriele Caviglioli and Tullio Florio. Under review.

Communications at Conferences

Oral communications:

- 1) "Development of a radiopharmaceutical for the detection of early atheromatous lesions", Advanced School in nanomedicine (25-28 September 2017, Pula, Sardinia).

Poster Communications:

- 1) "Injectable formulations for local administration of metformin hydrochloride", XXIII National Meeting in Medicinal Chemistry (6-9 September 2015, Campus University of Salerno, Fisciano).
- 2) "Study of Chitosan-Clodronate nanoparticles embedded in a thermoreversible gel based poloxamero", XV edition of Summer School in Pharmaceutical-Technological disciplines (9-11 September 2015, Campus of Fisciano, Department of Pharmacy).

- 3) "Development of gel formulations for localized release of metformin", 4-7 April 2016, 10^o World Meeting on Pharmaceutics, Biopharmaceutics and Pharmaceutical Technology, Glasgow (UK).
- 4) "Norbiotinamine as coupling agent for pretargeting: improvement of preparative reaction (optimization)", 5-8 September 2016, University of Calabria, Arcavacata di Rende (CS).
- 5) "Buccoadhesive polymeric films for oromucosal oxycodone delivery in acute pain control", 5-8 September 2016, University of Calabria, Arcavacata di Rende (CS).
- 6) "Optimization of a parenteral thermoresponsive formulation based on metformin hydrochloride", 3-4 April 2017, 2nd European Conference on Pharmaceutics: Novel Dosage Forms, Innovative Technologies.
- 7) "Preformulation study of multilayer films for local treatment of oral disease", Advanced School in nanomedicine, 25-28 September 2017, Pula, Sardinia.

Congresses Attended

- 1) XXIII National Meeting in Medicinal Chemistry (6-9 September 2015, Campus University of Salerno, Fisciano).
- 2) 10^o World Meeting on Pharmaceutics, Biopharmaceutics and Pharmaceutical Technology (4-7 April 2016, Glasgow, UK).
- 3) 2nd European Conference on Pharmaceutics: Novel Dosage Forms, Innovative Technologies (3-4 April 2017, Cracovia).

Courseware

Courses attended and passed (12 credits)

Courses Given by Teachers of the Department of Pharmacy (University of Genoa)

- 1) Multivariate analysis of chemicals data (Teachers: Lanteri, Armanino, Leardi) (3 credits)
- 2) Molecular markers of food quality and genuineness (Teachers: Boggia, Zunin) (2 credits)
- 3) Application of RAMAN spectroscopy to materials (Teachers: Carnasciali) (3 credits)
- 4) Innovative pharmaceutical dosage forms: preparation and control methods (Teachers: Russo, Parodi, Caviglioli, Baldassari, Zuccari) (2 credits)
- 5) Instrumental techniques for trace elements determination in pharmaceuticals, food products and environmental samples (Teachers: Minganti, Drava) (2 credits)

Courses Given by invited experts:

- 1) "Solid State Modification: Principles and Applications for Drug Solubility Enhancement", Dr. Paolo Gatti (DIFAR 07/11/2014).
- 2) "New trends in computer aided drug design", Dr. Tiziano Tuccinardi (DIFAR 09/12/2014).
- 3) "Elements of forensic chemistry", Dr. Narizzano Riccardo e Drs. Risso Fulvia, ARPAL (DCCI 18-19/05/2015).
- 4) "NIR spectroscopy: theory and application", dr. Tiziana Cattaneo e dr. Roberto Giangiacomo (DIFAR 29/02/2016).

National and International Schools or Workshops

- 1) XV Summer School in Pharmaceutical-Technological disciplines (9-11 September 2015, Campus di Fisciano, Department of Pharmacy).
- 2) Il Corso permanente di aggiornamento per i dottorandi del settore tecnologico-farmaceutico (5-8 September 2016, University of Calabria, Arcavacata di Rende, CS).
- 3) Advanced School in nanomedicine (25-28 September 2017, Pula, Sardinia).
- 4) Summer School "Tropi-Call Plus"-2017 (2-6 October 2017, University of Pisa).

Seminars Given

- 1) "Imaging in Oncology", (DIFAR 18/10/2017)

Seminars Attended

- 1) "Biocatalysis: applications in pharmaceutical synthesis", Dr. Matteo Massa, (DIFAR 28/11/2014).
- 2) "Natural molecules and Xeno-hormesis", Dr. Giacomo Mele, (DIFAR 28/11/2014).
- 3) "Alternative methods to animal testing", Drs. Benedetta Pollarolo, (DIFAR 28/11/2014).
- 4) "Recent aspects of therapeutic interest in the process of tumor metastasis", Drs. Camilla Zibana, (DIFAR 28/11/2014).
- 5) "The authorization process of medicines in Italy", Dr. Domenico Valle, Director Regulatory and PRA, Eli Lilly Italia, (DIFAR 10/04/2015).
- 6) "Neurons from stem cell: cognitive and clinical prospects in neurology", Sen. Elena Cattaneo, (Auditorium CBA 24/04/15).
- 7) "Therapeutic angiogenesis: vascular biology to regenerative medicine", Dr. Andrea Banfi, University Hospital Basel (CH), (DIMI 22/05/2015).
- 8) "Models for the in vitro study of human metabolism", Prof. Arti Ahluwalia, (Polo Alberti 16/07/15).
- 9) "The Biotin-(Strept)avidin system in pretargeting and in biotechnological applications", Drs. Irene Croce, (DIFAR 27/11/2015).
- 10) "Advanced technologies for the development of physiologically relevant in vitro alternative models", Jenia Dainalova, (DIFAR 27/11/2015).
- 11) "Palladium-catalyzed reactions: a revolutionary impact in Medicinal Chemistry", Andrea Desogus, (DIFAR 27/11/2015).
- 12) "Revolution in the treatment of parasitic diseases: Artemisinin as great scientific goal", Cinzia M. Francini, (DIFAR 27/11/2015).
- 13) "Druglikeness and related scoring methods: Ligand Efficiency and Lipophilic Ligand Efficiency", Sara Guariento, (DIFAR 27/11/2015).
- 14) "Odors, perfumes and pheromones as olfactory chemical mediators", Chiara Lacapra, (DIFAR 18/11/2016).
- 15) "Tuberculosis and other lung diseases: state of the art and recent therapeutic developments", Elda Meta, (DIFAR 18/11/2016).
- 16) "Play dirty: PAINS and promiscuous compounds", Anita Parricchi, (DIFAR 18/11/2016)
- 17) "Il marketing cosmetico: dalla mission aziendale alla risposta del consumatore", Silvia Rum, (DIFAR 18/11/2016)
- 18) "The vaccines: from the origins to the present day", Monica Sanna, (DIFAR 18/10/2017).

- 19) "Chronic Obstructive Pulmonary Disease (COPD): a pathology overview and the possible effects of Particulate Matter (PM)", Daniele Brignole, (DIFAR 18/10/2017).
- 20) "Depression: new therapeutic strategies" Mohamed Sadeghi (DIFAR 18/10/2017).
- 21) "Probiotics: properties, uses and interaction with human gut microbiome" (DIFAR 18/10/2017).

Other Activities

- 1) Laboratory assistance in Technology, Socioeconomy and Pharmaceutical Legislation II (CTF), 30 hours, a.a. 2015/2016 (first semester).
- 2) Laboratory assistance in Technology, Socioeconomy and Pharmaceutical Legislation II (CTF), 30 hours, a.a. 2016/2017 (first semester).



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



Curriculum: Scienze Farmaceutiche, Alimentari e Cosmetologiche

MOHAMMADREZA SADEGHI

Start of the Doctorate Program *November 1st, 2014*

End of the Doctorate Program *31 Ottobre 2017*

Advisors

Prof. Bruno Tasso

Thesis Title

"Synthesis of quinolizidine and benzoazole derivatives endowed with potential pharmacological activity"

Thesis abstract

During my PhD, I continued my research lines on chemical modifications of alkaloids derivatives, in order to create new molecules with potential antiproliferative activity. My work started with the synthesis of quinolizidine alkaloids, particularly lupinine and cytisine, for the preparation of compounds endowed with potential therapeutic interest, and particularly antiparasitic (against *Leishmania tropica* and *Leishmania infantum*), and anticholinesterase activity; I also used the pyrrolizidinic alkaloid laburnine as a starting compound, to compare the quinolizidine and pyrrolizidinic derivatives' activities. The quinolizidine nucleus, indeed, is a chemical moiety that has been widely used to synthesize new molecules (as described in literature), due to its well known biological activities; quinolizidine alkaloids are also very suitable for the linkage to other chemical moiety, such as carbo- and heterocyclic systems. Therefore I synthesized new N-alkyl and N-alkylarylcytisine derivatives, new basic molecules and some corresponding quaternary ammonium salts. In order to establish the possible influence of the length of the alkyl chain and the corresponding increase of lipophilicity on biological activity, I prepared the N-tetradecyl and N-hexadecylcytisine. I have also decided to prepare the quaternary ammonium derivatives, since S-alkylthiolupinine derivatives, prepared by other authors, after transformation into the corresponding quaternary ammonium salts, have shown a marked increase of antiparasitic activity. All these compounds showed a weak antiparasitic activity. Several quinolizidine derivatives of bi- and tricyclic aromatic rings, such as acridines, thioxanones, naphthoquinones and anthraquinones, bearing residues derived from lupinine, aminolupinane and thiolupinine, showed high inhibitory activity on acetylcholinesterase and butyrylcholinesterase. For this reason I have synthesized new lupinine, aminolupinane and thiolupinine derivatives of xanthene-9-carboxylic acid and new cytisine derivatives of 1,4-

naphthoquinone and anthraquinone. All synthesized compounds exhibited high inhibitory activity versus AchE and BuChE. The values of IC_{50} are in low micromolar or submicromolar concentration range. For some compounds also a moderate selectivity for one enzymes is been reached. In parallel with this research line, I also developed an interest towards benzotriazolic derivatives: the benzotriazole nucleus is largely explored due to its broad spectrum of biological activities including antiviral, antimicrobial and anticancer properties. For these reasons I synthesized benzotriazole 3,4,5-trimethoxybenzoate esters endowed with interesting antiproliferative activity (IC_{50} submicromolar). Besides a small series of 1-substituted benzoylbenzotriazoles (eight compounds), I design and synthesized a series of 28 benzoic esters of 1-(2,3-hydroxyalkyl) benzotriazoles. Moreover, I also focused on another alkaloyd, colchicine, well known for its antimitotic activity and its antitumoral potential (not yet exploited because of its disadvantages in therapy such as a very high toxicity). Both colchicine and the benzotriazole nucleus, then, could be exploited for their anticancer activities, after some chemical modifications. Therefore, in order to obtain compounds with improved anticancer activities, I synthesized a series of eight novel colchicine derivatives characterized by substituted 1,2,3-benzotriazoles moieties. Since colchicine exerts its activity by binding to a site localized in β -tubulin and thus achieving a conformational change in the tubulin dimer, I carried out docking simulations on the synthesized compounds, in order to predict their linkage to the β -tubulin. In comparison with the x-ray structure of colchicine bound to tubulin, the new synthesized compounds showed a different orientation in the binding sites but the calculated K_i values appeared to be in the nanomolar or subnanomolar concentration range, and one of them in particular was endowed with a lower K_i value than colchicine. Future *in vitro* assays will be carried out to validate the calculations that will be used to design novel analogues.

ACTIVITY REPORT

Research Activity

The research activity was mainly carried out at the IIT
Please indicate here if you have spent research periods in foreign countries.

Scientific Publications

Original publications on ISI Journals:

M. Sadeghi, M. Viale, I. Maric, B. Tasso, Synthesis of novel 3,4,5-trimethoxybenzoate of benzotriazole derivatives endowed with antiproliferative activity. *Bioorg. & Med. Chem.* Submitted

Communications at Conferences

Oral communications:

Poster Communications:

M. Sadeghi, M. Catto, B. Tasso, F. Novelli, M. Tonelli, A. Carotti, F. Sparatore, Synthesis of cytosine of quinones as potential cholinesterase inhibitors for Alzheimer's disease treatment. Giornate Italo-Francesi di Chimica, 25 – 26 Aprile 2016, Avignon, France

M. Sadeghi, A. Spallarossa, B. Tasso, Synthesis and preliminary docking studies of new colchicine-benzotriazole hybrid compounds. 3° International Conference on Drug Discovery & Designing, Austria

Congresses Attended

Giornate Italo-Francesi di Chimica, 25 – 26 Aprile 2016, Avignon, France

13° International Conference and Exhibition on Nanomedicine and Pharmaceutical Nanotechnology, Italy

3° International Conference on Drug Discovery & Designing, Austria

Courseware

Courses attended and passed (6 credits)

CORSO TIPO B :

- 1) Marker molecolari della qualità e della genuinità degli alimenti. Prof.ssa Zunin e Prof.ssa Boggia
- 2) Progettazione e sviluppo di inibitori di proteina-chinasi come nuovi agenti antitumorali. Prof.ssa Schenone
- 3) Ricerca bibliografica e brevettuale nelle scienze farmaceutiche tramite banche dati. Prof.ssa Brullo e Fossa
- 4-) metodi di preparazione e controllo di forme farmaceutiche innovative.
Prof.Baldassari&caviglioli&Russo&Parodi
- 5-) Nomenclatura INN ed IUPAC di farmaci a struttura organica.
Prof.Grossi
- 6-) Tecniche strumentali per la determinazione di elementi in traccia di interesse farmaceutico, alimentare, ambientale.
Prof.Minganti&Dreva

CORSO TIPO A :

- 1) "New trends in computer aided drug design". Prof. Tiziano Tuccinardi
- 2) Elementi di chimica forense. Dott.ssa Risso Fulvia e Dott.Narizzano Riccardo
- 3) Medicinal chemistry with carbohydrates: the influenza virus and the discovery of sialidase inhibitors" Prof.ssa Anna Bernardi (Università di Milano)

Courses Given by invited experts:

National and International Schools or Workshops

- 1) Corso di spettrometria di massa ,Siena Certosa di Pontignano 12-18 Marzo 2016.
- 2) Riunione Nazionale "A. Castellani" dei Dottorandi di Ricerca in Discipline Biochimiche

Seminars Given

Depression and new therapeutic strategies

Seminars Attended

- 1) Hsp 90 nella terapia antitumorale al disegno di nuovi inibitori allosterici (Dott.gerolamo vettoretti 25/05/2015)
- 2) Biocatalisi: applicazioni in sintesi farmaceutica (Dr. Matteo Massa 01/12/14) .
- 3) Molecole naturali e Xeno-ormesi (Dr Giacomo Mele 01/12/14)
- 4) Metodi alternativi alla sperimentazione animale (Dr.ssa Benedetta Pollarolo 01/12/14)
- 5) Recenti aspetti d'interesse terapeutico del processo di metastasi tumorale (Dr.ssa Camilla Zibana 01/12/14)
- 6) Ruolo della sfingosina-1-fosfato e della sfingosina kinasi nella polarizzazione di linfociti TH17 umani (Prof.Raffaele de Palma 16/12/2014)
- 7) Chemometrics in proteomics studies(Prof.Beata Walczac 22/01/2016)
- 8) Il sistema biotina-(strept)avidina nel pretargeting e in applicazioni biotecnologiche(Dott.ssa Irene Croce 27/11/2015)

- 9) Tecnologie avanzate per lo sviluppo di modelli alternativi fisiologicamente rilevanti in vitro(Dott.ssa Jenia Danailova 27/11/2015)
- 10) Reazioni Palladio-catalizzate: un impatto rivoluzionario in Chimica Farmaceutica(Dott. Andrea Desogus 27/11/2015)
- 11) Rivoluzione nella terapia delle malattie parassitarie: Artemisinina come grande successo scientifico.(Dott.ssa Cinzia M. Francini 27/11/2015)
- 12) -) Druglikeness e metodi di score relativi: Ligand Efficency e Lipophilic Ligand Efficency.(Dott.ssa Sara Guariento 27/11/2015)
- 13) -) Analisi esplorativa multivariata: applicazioni al di fuori del laboratorio.(Dott. Remo Simonetti 27/11/2015)
- 14) Chemometrics in proteomics studies(Prof.Beata walczak ,università di Silesian 22/02/2016)
- 15) Il marketing cosmetico: dalla mission aziendale alla risposta del consumatore.(Dr.ssa Silvia Rum)
- 16) Odori, profumi e feromoni come mediatori chimici olfattivi.(Dr.ssa Chiara Lacapra)

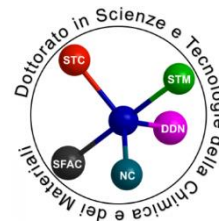
- 17) Giocare sporco: PAINS e composti promiscui.(Dr.ssa Anita Parricchi)
- 18) Tubercolosi ed altre patologie polmonari: stato dell'arte e recenti sviluppi terapeutici.(Dr.ssa Elda Meta)
- 19) The vaccines: from the origins to the present day.(Sanna Monica)
- 20) hronic Obstructive Pulmonary Disease (COPD): a
- 21) pathology overview and the possible effects of Particulate Matter (PM).(Brignole Daniele)
- 22) Imaging in Oncology.(Pastorino Sara)
- 23) 3D printing and biofabrication.(Yan Mengying)
- 24) Probiotics: properties, uses and
- 25) interaction with human gut microbiome.(Turrini Federica)

OtherActivities

- 1) Tutor didattico in “Anatomia umana” per studenti dei corsi di Laurea in Farmacia e Chimica e Tecnologie Farmaceutiche.(2015/16)
- 2) Assistenza di supporto alla didattica nell’insegnamento “Analisi Strumentale dei Farmaci” – corso di Laurea in Chimica e Tecnologie Farmaceutiche.(2015/16)
- 3) Tutor didattico in “Anatomia umana” per studenti dei corsi di Laurea in Farmacia e Chimica e Tecnologie Farmaceutiche.(2016/17).
- 4) Tutor didattico in “Chimica Analitica” per studenti dei corsi di Laurea in Farmacia e Chimica e Tecnologie Farmaceutiche.(2016/17) .
- 5) Assistenza di supporto alla didattica nell’insegnamento “Analisi dei medicinali II” – corso di Laurea in Chimica e Tecnologie Farmaceutiche.(2016/17).



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



Curriculum: Pharmaceutical, Food and Cosmetic Sciences
(XXX cycle)

MONICA SANNA

Start of the Doctorate Program *November 1st, 2014*

End of the Doctorate Program *October 31st, 2017*

Advisors *Prof. Silvia Schenone*

Thesis Title

Design, synthesis and biological evaluation of pyrazolo-pyrimidine and related isosteres as inhibitors of protein kinases, potential antineoplastic agents.

Thesis abstract

The protein kinase enzyme family is one of the largest super-families of homologous proteins and are responsible for modifying an estimated one third of the human proteome. These enzymes catalyze the transfer of the terminal phosphate group of ATP to a hydroxyl group of serine, threonine or tyrosine present in a target protein. Depending on the substrate, protein kinases can be classified into serine-threonine kinases and tyrosine kinases.

According to their cellular location, both classes can be further divided into receptor kinases (located in the cell membrane) or cytoplasmic kinases (located within the cell).

Protein kinases are key regulators of cell functions. They direct the activity, localization and other functions of many proteins, and serve to orchestrate the activity of almost all cellular processes. It has also been firmly demonstrated that kinase activity alterations, leading to the disruption of cell signaling cascades, play important roles in many diseases, including cancer, inflammation, neurological disorders and diabetes. For all these reasons, kinases represent important targets for drug therapy. It is estimated that over 30% of the drug discovery efforts in pharmaceutical and biotech companies are directed towards finding and validating protein kinase inhibitors.

My PhD project was aimed at synthesizing inhibitors of the tyrosine kinases Src, Fyn and Hck and the serine-threonine kinase SGK-1.

Src family kinases are a group of highly homologous non receptor tyrosine kinases that are involved in the regulation of several phases of cell life (e.g. growth, differentiation, apoptosis). The hyperactivation of c-Src, a member of this family of enzymes, has been proved to be closely connected with the development and progression of several tumor types. In this context, the research group where I worked has synthesized a large library of pyrazolo[3,4-*d*]pyrimidines; many of these molecules resulted to be nanomolar inhibitors of the cytoplasmic tyrosine kinase c-Src. This family of compounds also showed a good antiproliferative

activity against several cancer cell lines: neuroblastoma, chronic myeloid leukaemia, rhabdomyosarcoma, osteosarcoma, prostate cancer, and mesothelioma. Important results have been obtained in several mouse models of cancer.

Recently, c-Src has been shown to be frequently hyperactivated or overexpressed also in glioblastoma, a brain tumour characterized by a high degree of proliferation, angiogenesis, necrosis, and invasiveness. Src inhibition reduced glioblastoma cell growth, viability and migration both *in vitro* and in mouse models. In this context, I synthesized a library of pyrazolo[3,4-*d*]pyrimidines; some of these compounds demonstrated a good activity towards Src in enzymatic assays and on different glioblastoma cell lines.

At the same time, the pyrrolo[2,3-*d*]pyrimidine scaffold is also being extensively investigated and in the last few years many of such compounds resulted active as kinase inhibitors. For this reason I synthesized a family of pyrrolo[2,3-*d*]pyrimidines which have been tested on Src in enzymatic assays and as antiproliferative agents on a specific cancer cell line.

Fyn is another member of Src family kinases and it phosphorylates a variety of target proteins involved in different signaling pathways. To date, the implication of Fyn in solid and in hematologic malignancies has become more evident and its abnormal activity has been shown to be related to severe central nervous system pathologies such as Alzheimer's and Parkinson's disease.

The research group where I worked synthesized a library of pyrazolo[3,4-*d*]pyrimidines active as Fyn inhibitors endowed with K_i values in the nanomolar range. Some of these compounds inhibited the phosphorylation of the protein Tau in an Alzheimer's model cell line and showed antiproliferative activities against different cancer cell lines. On the basis of these interesting results, I decided to expand the structure-activity relationship (SAR) on this family of inhibitors and planned the synthesis of new compounds.

Hematopoietic cell kinase (Hck) is another member of Src family kinases and it is expressed in hematopoietic cells, particularly myelomonocytic cells and B lymphocytes. High levels of Hck are involved in chronic myeloid leukemia and in other hematologic tumors, but its activity is also connected with viral infections, including HIV-1. In this context, our research group developed a docking study to identify new Hck inhibitors. We screened some molecules of our *in house* library of pyrazolo[3,4-*d*]pyrimidines and some commercial compounds, and we tested, in enzymatic and cellular assays, the most promising compounds which have showed an activity towards Hck in the low micromolar range. On the basis of these results, I synthesized some new pyrazolo[3,4-*d*]pyrimidines, analogues of the most active inhibitors, and some derivatives of the commercial compound, which showed the best Hck inhibitory activity, in detail 5,6,7,8-tetrahydro[1]benzothieno[2,3-*d*]pyrimidine molecules. Enzymatic assays of these compounds are still in progress.

SGK-1 is a member of the serum- and glucocorticoid-regulated kinase family that is involved in antiapoptotic functions and in the regulation of cell survival, proliferation, and differentiation. A pivotal role of SGK-1 in carcinogenesis and in resistance to anticancer therapy has been suggested. For all these reasons, we decided to developed an *in silico* screening in order to see if some our pyrazolo[3,4-*d*]pyrimidines, already active as Src and/or Abl inhibitors, were also active towards SGK-1. One of these compounds showed a very interesting activity. On the basis of these interesting results, I synthesized a library of pyrazolo[3,4-*d*]pyrimidines, analogues of the most active compounds, in order to develop a lead optimization study. Other synthesis and biological studies are in progress.

During the third year of my PhD I also spent a research period at the School of Pharmacy of the University of Nottingham under the supervision of Prof. Cameron Alexander. In these months, I developed a high-throughput screening process by using a 2D Inkjet printer in order to identify the best polymeric carrier able to solubilize in water some different representative pyrazolo[3,4-*d*]pyrimidine derivatives using as little of the sample as possible. I choosed five compounds of our in-house library of pyrazolo[3,4-*d*]pyrimidines

and I synthesized a new analogue. Then I combined these derivatives with seven different hydrophilic commercial available polymers, that are able to inhibit crystallization and to create an amorphous solid dispersion. This new technique represents an efficient method to evaluate pharmaceutical formulations, since it uses a nanogram quantity of materials which is three-six fold lower than the amount used with conventional methods. Amorphous solid dispersions have broadly adopted for the dosage of oral dispersions that result intrinsically suitable for chemotherapeutic drugs as mentioned above.

ACTIVITY REPORT

Research Activity

Research Period Abroad

27.03.2017-28.07.2017 School of Pharmacy, University of Nottingham. Supervisor: Prof. Cameron Alexander.

Scientific Publications

1. Musumeci, F.; Schenone, S.; Grossi, G.; Brullo, C.; Sanna, M. Analogs, formulations and derivatives of imatinib: a patent review. *Expert Opin Ther Pat.* **2015**, *25*, 1411-1421.
2. Musumeci, F.; Sanna, M.; Grossi, G.; Brullo, C.; Fallacara, A.L.; Schenone, S. Pyrrolo[2,3-*d*]pyrimidines as kinase inhibitors. *Curr Med Chem.* **2017**, *24*, 2059-2085.
3. Musumeci, F.; Sanna, M.; Greco, C.; Giacchello, I.; Fallacara, A.L.; Amato, R.; Schenone, S. Pyrrolo[2,3-*d*]pyrimidines active as Btk inhibitors. *Expert Opin Ther Pat.* **2017**, Jul 20, 1-14.
4. Sanna, M.; Sicilia, G.; Alazzo, A.; Singh, N.; Musumeci, F.; Schenone, S.; Spriggs, K.; Burley, J.; Taresco, V.; Alexander, C. Water solubility enhancement of pyrazolo[3,4-*d*]pyrimidine scaffold derivatives via miniaturized polymer-drug blends microarrays. Manuscript submitted.

Communications at Conferences

Poster Communications:

1. Musumeci, F.; Sanna, M.; Desogus, A.; Brullo, C.; Tintori, C.; Botta, M.; Indovina, P.; Giordano, A.; Schenone, S. "Synthesis of pyrazolo[3,4-*d*]pyrimidine derivatives active in a preclinical glioblastoma model". XXIII National Meeting on Medicinal Chemistry - 9th Young Medicinal Chemists Symposium, Campus di Fisciano, Università degli Studi di Salerno, 6-9/09/2015.
2. Musumeci, F.; Sanna, M.; Giacchello, I.; Mazzei, M.; Schenone, S. "Synthesis of heterocyclic compounds to be tested as potentiators or correctors of mutant CFTR in cystic fibrosis". VI European Workshop in Drug Synthesis, Certosa di Pontignano, Siena, 15-19/05/16.
3. Molinari, A.; Musumeci, F.; Tintori, C.; Brullo, C.; Sanna, M.; Schenone, S.; Botta, M. "Synthesis of a new generation of Hck inhibitors: a hit to lead optimization study". VI European Workshop in Drug Synthesis, Certosa di Pontignano, Siena, 15-19/05/16.
4. Graco, C.; Sanna, M.; Musumeci, F.; Giacchello, I.; Perrotti, N.; Alcaro, S.; Ortuso, F.; Schenone, S. "Synthesis of a new generation of pyrazolo[3,4-*d*]pyrimidines as SGK-1 inhibitors". 17th Hellenic Symposium on Medicinal Chemistry, Thessaloniki, 1-3/06/17.
5. Sanna, M.; Greco, C.; Musumeci, F.; Giacchello, I.; Schenone, S.; Fallacara, A.L.; Trist, I.M.; Botta M. "Synthesis of a

new generation of pyrazolo[3,4-d]pyrimidines as Fyn inhibitors". XXVI Congresso Nazionale della Società Chimica Italiana, Paestum, Salerno, 10-14/09/2017.

6. Giacchello, I.; Musumeci, F.; Greco, C.; Sanna, M.; Schenone, S.; Trincavelli, M.L.; Tuccinardi, T. "Substituted pyrazolo[3,4-b]pyridines as potent A1 adenosine antagonists". XXVI Congresso Nazionale della Società Chimica Italiana, Paestum, Salerno, 10-14/09/2017.

Congresses Attended

1. XXIII National Meeting in Medicinal Chemistry - 9th Young Medicinal Chemists Symposium (XXIII NMMC-NPCF9) Campus di Fisciano, Università degli Studi di Salerno, 06-09/09/2015.
2. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum, Salerno, 10-14/09/2017.

Courseware

Courses attended and passed (9 credits)

Courses Given by Teachers of the Unige and IIT:

- 1) "Biotecnologie farmaceutiche". Prof. Mauro Mazzei (3 credits).
- 2) "Progettazione e sviluppo di inibitori di proteina-chinasi come nuovi agenti antitumorali". Prof. Silvia Schenone (2 credits).
- 3) "Patent and bibliographic databases searching in medicinal chemistry". Proff. Paola Fossa and Chiara Brullo (2 credits).
- 4) "Instrumental techniques for trace elements determination in pharmaceuticals, food products and environmental samples". Proff. Vincenzo Minganti and Giuliana Drava (2 credits).

Courses Given by invited experts:

- 1) "New trends in computer aided drug design". Prof. Tiziano Tuccinardi, University of Pisa (09/12/2014).
- 2) "X-ray based experimental techniques and characterization of nano-materials". Prof. Alberto Morgante, CNR-IOM and Physics Department Trieste University (31/03/2015).
- 3) "Yb and Eu strongly correlated electron systems". Dr. Ivan Curlik, University of Presov, Slovacchia (21-22/04/2015).
- 4) "Elementi di Chimica Forense". Dr. Narizzano Riccardo e Dr. Risso Fulvia, ARPAL, Genova (18-19/05/2015).
- 5) "Medicinal chemistry with carbohydrates: the influenza virus and the discovery of sialidase inhibitors". Prof. Anna Bernardi, University of Milan (13/11/15).

Seminars attended

- 1) "Biocatalisi: applicazioni in sintesi farmaceutica". Dr. Matteo Massa, University of Genoa (28/11/2014).
- 2) "Molecole naturali e Xeno-ormesi". Dr. Giacomo Mele, University of Genoa (28/11/2014).
- 3) "Metodi alternativi alla sperimentazione animale". Dr. Benedetta Pollarolo, University of Genoa (28/11/2014).
- 4) "Recenti aspetti d'interesse terapeutico del processo di metastasi tumorale". Dr. Camilla Zigana, University of Genoa (28/11/2014).
- 5) "Recent cosmetic science and formulation technology". Prof. Yuji Yamashita, Pharmaceutical and Life Science Dept. Chiba Institute of Science (03/03/2015).
- 6) "Bioenergetica dei tumori". Prof. Alessandro Morelli, University of Genoa (05/03/2015).
- 7) "Il processo autorizzativo dei farmaci in Italia". Dr. Domenico Valle, Direttore Regulatory and PRA, Eli Lilly Italia (10/04/2015).
- 8) "Hsp90 nella terapia antitumorale: dall'analisi conformazionale al disegno di nuovi inibitori allosterici". Dr. Gerolamo Vettoretti, Istituto di Chimica del Riconoscimento Molecolare -CNR (25/05/2015).
- 9) "The Biotin-(Strept)avidin system in pretargeting and in biotechnological applications". Dr. Irene Croce, University of Genoa (27/11/15).
- 10) "Advanced technologies for the development of physiologically relevant in vitro alternative models". Dr. Jenia Danailova, University of Genoa (27/11/15).
- 11) "Palladium-catalyzed reactions: a revolutionary impact in Medicinal Chemistry". Dr. Andrea Desogus, University of Genoa (27/11/15).
- 12) "Revolution in the treatment of parasitic diseases: Artemisinin as great scientific goal". Dr. Cinzia M. Francini, University of Genoa (27/11/15).
- 13) "Druglikeness and related scoring methods: Ligand Efficiency and Lipophilic Ligand Efficiency". Dr. Sara Guariento, University of Genoa (27/11/15).
- 14) "Chemometrics in proteomics studies". Prof. Beata Walczak, Institute of Chemistry, Silesian University, Katowice, Poland (22/01/16).
- 15) "I nutraceutici. I farmaci per le persone sane". Prof. Ettore Novellino, University of Naples (26/01/16).
- 16) "Il marketing cosmetico: dalla *mission* aziendale alla risposta del consumatore". Dr. Silvia Rum, University of Genoa (18/11/16).
- 17) "Odori, profumi e feromoni come mediatori chimici olfattivi". Dr. Chiara Lacapra, University of Genoa (18/11/16).
- 18) "Giocare sporco: PAINS e composti promiscui". Dr Anita Parricchi, University of Genoa (18/11/16).
- 19) "Tubercolosi ed altre patologie polmonari: stato dell'arte e recenti sviluppi terapeutici". Dr. Elda Meta, University of Genoa (18/11/16).
- 20) "Chronic Obstructive Pulmonary Disease (COPD): a pathology overview and the possible effects of Particulate Matter (PM)". Dr. Daniele Brignole, University of Genoa (18/10/17).
- 21) "Imaging in Oncology". Dr. Sara Pastorino, University of Genoa (18/10/17).

- 22) "Depression: new therapeutic strategies". Dr. Mohamed Sadeghi, University of Genoa (18/10/17).
- 23) "Probiotics: properties, uses and interaction with human gut microbiome". Dr. Federica Turrini, University of Genoa (18/10/17).

Seminars given

"The vaccines: from the origins to the present day". University of Genoa (18/10/17).

National and International Schools or Workshops

1. VI European Workshop in Drug Synthesis, Certosa di Pontignano, Siena (15-19/05/16).
2. European School of Medicinal Chemistry, Campus "Collegi del Colle e Tridente", Urbino (26/06/16-01/07/16).
3. Computer-Aided Drug Design-Summer School, Dipartimento di Farmacia, Pisa (11-16/07/16).

Other Activities

- 1) Laboratory assistant at the course of "Analisi dei medicinali II" (Prof. Chiara Brullo), for the third year students of the "Chimica e Tecnologia Farmaceutiche" course, University of Genoa. (Academic year 2015/2016).
- 2) Teaching tutor of "Chimica Fisica" and "Chimica Organica" for the second year students of the "Farmacia" and "Chimica e Tecnologia Farmaceutiche" courses, University of Genoa. (Academic year 2015/2016).
- 3) Laboratory assistant at the course of "Analisi dei medicinali I" (Prof. Michele Tonelli), for the second year students of the "Chimica e Tecnologia Farmaceutiche" course, University of Genoa. (Academic year 2016/2017).
- 4) Teaching tutor of "Chimica Organica" for the second year students of the "Farmacia" and "Chimica e Tecnologia Farmaceutiche" courses, University of Genoa. (Academic year 2016/2017).

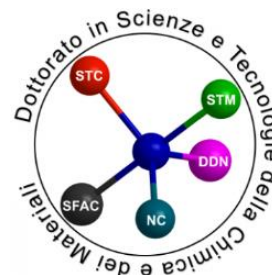


Università degli Studi di Genova

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

Curriculum: NAnoChemistry

Javad Shamsi



Start of the Doctorate Program *November 1st, 2014*

End of the Doctorate Program *October 31st, 2017*

Advisors

Prof. A. Saccone (UniGe)

Prof. L. Manna (IIT)

Thesis Title:

Colloidal Synthesis of Lead Halide Perovskite Nanocrystals for Optoelectronic Application

Thesis abstract:

My research is mainly focused on the synthesis of lead halide perovskite nanocrystals (LHP NCs). Compared with bulk materials, the quantum yields of LHP NCs reach up to 90%, making them particularly attractive for display application. The properties of LHP NCs are highly dependent on their size and shape, as has been demonstrated for different shapes during my second year of PhD, such as nanoplatelets, nanosheets, nanowires. However, some challenges remain in this field in order to exploit such materials in optoelectronic applications. One problem with the hot injection synthesis of these NCs (the standard method) is that both nucleation and growth occur swiftly. Critical steps of this synthesis scheme are the fast injection of a preheated solution of cesium oleate and a fast cooling that follows immediately after that, which makes it hard to control their size, upscale the process and more in general to test variants in a reproducible fashion. In addition, this method does not yield NCs in quantities sufficient for their implementation in optoelectronic devices. Despite the excellent photoluminescence quantum yield (PLQY) of LHP NCs in solution, preserving a high emission efficiency in the solid state is another issue that needs to be addressed. During my last year PhD, I have been trying to find novel routes which can address these issues. We here report two alternative approaches to synthesize LHP NCs (mainly CsPbX₃): 1) "heat up" method as a direct and "colloidal transformation" as an indirect approach. The heat up method results quantum-confined, blue-emitting CsPbX₃ (X: Cl, Br) nanoplatelets

(NPLs) that self-assemble into stacked lamellar structures and CsPbI₃ nanowires. This synthesis method can be easily scaled up to yield several grams of NPL products. In the second part, we report the synthesis of CsX NCs as colloidal precursors which enable us to transform them into the CsPbX₃ NCs at room temperature. Finally we fabricate green-emitting, all-solution-processed light-emitting diodes by using CsPbX₃ NC film as an active layer with an external quantum efficiency of 1.1% and a luminance of 590 Cd/m².

ACTIVITY REPORT

Research Activity

- The research activity was mainly carried out at the IIT

Research Period Abroad:

- ✓ **University of Oxford, Condensed Matter Physics, Prof Henry Snaith Lab; October 2017**

Scientific Publications:

- ✓ Low-Temperature Electron Beam-Induced Transformations of Cesium Lead Halide Perovskite Nanocrystals
Z Dang, **J Shamsi**, QA Akkerman, M Imran, G Bertoni, R Brescia, L Manna
ACS omega 2 (9), 5660-5665 2017
- ✓ Bright Emitting Perovskite Films by Large-Scale Synthesis and Photo-Induced Solid State Transformation of CsPbBr₃ Nanoplatelets
J Shamsi, P Rastogi, V Caligiuri, AL Abdelhady, D Spirito, L Manna, R Krahne
ACS nano 2017
- ✓ In Situ Transmission Electron Microscopy Study of Electron Beam-Induced Transformations in Colloidal Cesium Lead Halide Perovskite Nanocrystals
Z Dang, **J Shamsi**, F Palazon, M Imran, QA Akkerman, S Park, G Bertoni, L Manna
ACS nano 2017
- ✓ Hierarchical Multi-Shelled Nanoporous Mixed Copper Cobalt Phosphide Hollow Microspheres as a Novel Advanced Electrode for High-Performance Asymmetric Supercapacitors
SE Moosavifard, SK Kaverlavani, **J Shamsi**, A Bakouei
Journal of Materials Chemistry A 5 (35), 18429-18433 1 2017
- ✓ N-Methylformamide as a Source of Methylammonium Ions in the Synthesis of Lead Halide Perovskite Nanocrystals and Bulk Crystals
J Shamsi, AL Abdelhady, S Accornero, M Arciniegas, L Goldoni, L Manna
ACS energy letters 1 (5), 1042-1048 8 2016
- ✓ Colloidal Synthesis of Strongly Fluorescent CsPbBr₃ Nanowires with Width Tunable Down to the Quantum Confinement Regime
M Imran, F Di Stasio, Z Dang, C Canale, AH Khan, **J Shamsi**, R Brescia, L Manna
Chemistry of Materials 28 (18), 6450-6454 28 2016

- ✓ Colloidal Synthesis of Quantum Confined Single Crystal CsPbBr₃ Nanosheets with Lateral Size Control Up to the Micrometer Range
J Shamsi, Z Dang, P Bianchini, C Canale, F Di Stasio, R Brescia, M Prato, L Manna
Journal of the American Chemical Society 138 (23), 7240-7243 82 2016
- ✓ All-Solid State, Flexible, High-Energy Integrated Hybrid Micro-Supercapacitors Based on 3D LSG/CoNi₂S₄ Nanosheets
SE Moosavifard, **J Shamsi**, MK Altafi, ZS Moosavifard
Chemical Communications 52 (89), 13140-13143
- ✓ Monodisperse CsX (X = Cl, Br, I) Nanocrystals as Colloidal Precursors to CsPbX₃ Nanocrystals
J Shamsi, Z Dang, P Ijaz, AL Abdelhady, I Moreels, L Manna
"Submitted"
- ✓ Solvent Acidolysis Crystallization of CH₃NH₃PbBr₃ Bulk Crystals for Enhanced Optoelectronic Properties
AL Abdelhady, S Dogan, F Palazon, D Altamura, S G Motti, **J Shamsi**, A Petrozza, C Giannini, R Krahn, L Manna
"Submitted"

Communications at Conferences

Oral communications:

2017, Oxford, UK. PSCO 2017

"A general method for the large-scale synthesis of uniform confined perovskite nanoplatelets and their solid state transformation"

Poster Communications:

1. 2016, Marburg, Germany. Nanax7.
"Nanometer-thick single-crystalline CsPbBr₃ perovskite nanosheets with micrometer-scale lateral size"
2. 2016, Genova, Italy. 2de International Conference on Perovskite Solar Cells and Optoelectronics (PSCO 2016).
"Quantum-confined single crystal CsPbBr₃ perovskite nanosheets with micrometer-scale lateral size"
3. 2017, Braga, Portugal. Nanax8.
"Chemical strategy towards hybrid lead halide perovskite: From bulk crystal to Nanocrystal"

Congresses Attended

2016, Genova, Italy. 12th Congress of the Interdivisional Group of Organometallic Chemistry

Courseware

During the PhD Javad Shamsi has acquired **xxx credits** of Courseware.

Courses attended and passed (19 credits)

- ✓ Opto-Electronic Properties of Semiconductor Quantum Dots **(1 credit)**
- ✓ Energy related applications of colloidal nanocrystals **(1 credit)**
- ✓ Characterization of functionalized and water soluble nanoparticles **(1 credit)**
- ✓ Basics of Crystallography **(1 credit)**

- ✓ X-rays based Characterization Techniques (1 credit)
- ✓ Electron microscopy (1 credit)
- ✓ Science and Technology of two-dimensional crystals (1 credit)
- ✓ Electrical and Raman characterization techniques (1 credit)
- ✓ Magnetism, magnetic properties and applications of magnetic nanoparticles (1 credit)
-
- ✓ Electronic Properties of Solids (type B: 3 credits)
- ✓ Characterization of polymer materials (6 credits)
- ✓ Conventional and Unconventional Superconductivity: An overview”, Prof. Ernst Bauer, Institute of Solid State Physics, Vienna University of Technology, Austria (9-11 November 2015, DCCI, Università di Genova, type A: 1 credit)

National and International Schools or Workshops

- ❖ June 12-18, 2016, Krutyn, Poland “XXth International Krutyn Summer School 2016”
Advanced Perovskite, Hybrid and Thin-film photovoltaics (XXX Credits)

Seminars Given (xxx Credits)

- 21.1.2016, iit, NACH group meeting; “CsPbBr₃ Perovskite Nanosheets”
- 23.5.2016, Gent university, Gent, Belgium “Zeger Hens” group meeting; “Shape controlling of CsPbBr₃ NCs”
- 24.1.2017, iit, Perovskite group meeting, “Colloidal Synthesis of Lead Halide Perovskite Nanocrystals”
- 18.5.2017, iit, Milan, Perovskite group meeting, “Large-Scale Synthesis and Photo-induced Solid State Transformation of CsPbBr₃ Nanoplatelets”
- 2 Seminars (annual presentation) at University “October 2015” and “October 2016”

Seminars Attended (24 seminars, 3 Credits)

1. “Field-effect transistor and solar cells made of individual colloidal PbS” Sedat Dogan, January 8th 2015
2. “Plasmonic Nanomaterials” Mehdi H. ,January 12th 2015
3. “Materials for Sodium batteries” Passerini S., January 16th 2015
4. “Design, fabrication and characterization of plasmonic structures for graphene-based devices and superresolution” Lotito V., January 19th 2015
5. “High energy Lithium ion and lithium sulfur batteries” Agostini M., February 20th 2015
6. “Using colloidal quantum dots to boost photovoltaic cell performance” Kazes M., February 25th 2015
7. “Versatile fabrication of highly porous cryogels from noble metal nanoparticles” Freytag A., March 4th 2015
8. “Structure-activity relationship in CO oxidation over bimetallic AuCu Nanocrystals: the role of nanocrystal size, composition and support interaction” Colombo M., March 18th 2015
9. “Control of surface chemistry of nanodiamonds for bio-application” J. C. Arnault, November 9th 2015
10. “Semiconductor nanocrystals: discovery, milestone and recent theoretical developments” Alexander L. Efros , November 20th. 2015
11. “Insight in the chemistry of metal sulfide nanocrystals and their application in photovoltaicsc” Peter Reiss, November 25th 2015
12. “Recent advances with FIB-milled microcavities” Lucas Flatten, January 19th 2016

13. *"Perovskites: an old material for the third generation of PV solar panels"* **Laura Miranda Perez**, April 21st 2016
14. *"Colloidal nanoparticles and applications"* **Antonios G. Kanaras**, April 28th 2016
15. *"Hydration induced spin glass state in a frustrated Na-Mn-O triangular lattice"* **Ioanna Bakaimi**, April 28th 2016
16. *"Spatio-temporal visualization of atomic motions in low-dimensional materials"* **Giovanni Maria Vancore**, May 3rd 2016
17. *"The power of intermolecular interactions in organic semiconductors: from threaded molecular wires to PCBM single crystals"* **Franco Cacialli**, May 5th 2016
18. *"First-principles predictions of substrate effects on silicone"* **Udo Schwingenschloegl**, May 9th 2016
19. *"Nano-photonic phenomena in van der waals heterostructures"* **Dmitri N. Basov**, June 8th 2016
20. *"Perovskite nanocrystals for optoelectronic application"* **Alexander Weber-Bargioni**, November 11th 2016
21. *"Colloidal double quantum dots"* **Dan Oron**, February 14th 2017
22. *"Synthetic methodology for colloidal nanomaterials: limitations and opportunities"* **Dmitri V. Talapin**, May 26th 2017
23. *"High-throughput design of doped colloidal nanocrystals"* **Emory Chan**, June 1st 2017
24. *"Perovskite nanocrystals - the new generation of defect tolerant luminescent materials"* **Sameer Sapra**, June 14th 2017

Other Activities

- **Visiting** the Zeger Hens lab, Gent University, Gent, Belgium (May 22nd 2016, 1 week)



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



Curriculum: Scienze e Tecnologie Chimiche e Scienza e
Tecnologia dei Materiali

Giulia_Torrielli

Start of the Doctorate Program *November 1st, 2014*

End of the Doctorate Program *November 1st, 2017*

Advisors

Prof. Maurizio Ferretti

Thesis Title

“Diagnostic investigation and physical- chemical procedures for the Cultural Heritage”.

Thesis abstract

The research aims to understand the reason why this change took place, by analyzing the decay and so discovering its causes through scientific studies; this research must focus to a constant development of the cultural heritage conservation techniques.

The investigation involves the study of porous materials behavior, contaminating compresses of commonly known materials in the restoration field, with a saline solution and then subjecting them to two different desalination treatment: wraps with adsorbent materials and an innovative patent method. The results will be compared with each other and an analysis of the material behavior after different treatments will be performed. The goal is to make the patented method applicable to several cases.

ACTIVITY REPORT
Research Activity

During the third year (in 2017), three-month research period was held at the University of Zaragoza (Spain).

Scientific Publications

Original publications on ISI Journals:

- 1) G. Torrielli, V. Caratto, L. Gaggero, M. Ferretti. *Innovative method and apparatus for deep cleaning of soluble salts from mortars and lithic materials*. Energy Procedia (2016 accepted).
- 2) G. Torrielli, A. Provino, M. Ferretti, P. Manfrinetti. *Instrumental characterization of gypsum from the Monterverde’s sculptures. A preliminary case study*. Journal of Cultural Heritage (submitted)
- 3) G.Torrielli, v.Caratto, S.Alberti, F.Fossati, M.Ferretti. A New method for paint cleaning (submitted)

Patent

- 1) International patent “*Apparatus and method for treating porous materials*”, G.Torrielli, L. Gaggero, M. Ferretti, n. PCT/IB2015/055129.

Communications at Conferences

Oral communications:

- 1) G. Torrielli, V. Caratto, F. Locardi, E. Sanguineti, L. Gaggero, G. Petrillo, M. Ferretti. *Removal of natural waxes deposit from artistic surfaces by means of TiO₂-NPs photocatalysis*. Sustainability in Cultural Heritage, CNR Rome, 11-12 January 2016.
- 2) G. Torrielli, V. Caratto, L. Gaggero, M. Ferretti. *Innovative method for remove soluble salts from mortars and lithic materials*. XVI Congresso Nazionale della Chimica dell'ambiente e dei beni culturali, Lecce 26-29 June 2016.
- 3) G. Torrielli, A.Provino, M.Ferretti, P.Manfrinetti. *Idealità e Materialismo, caratterizzazione strumentale dei gessi di Giulio Monteverde*. Bistagno, (AL), 8 July 2017.
- 4) G. Torrielli, A.Provino, M.Ferretti, P.Manfrinetti. *"Instrumental characterization of the gypsum from the Monteverde's sculptures"*. Giornata della Chimica Ligure, 20 October 2017.

Poster Communications:

- 1) "Studio del degrado fotocatalitico di cere naturali mediante impiego di TiO₂ nanometrico" – GIULIA TORRIELLI, V.Caratto, F.Locardi, E.Sanguineti, L.Gaggero, M.Ferretti. XV Congresso Nazionale Divisione di Chimica dell'Ambiente e Chimica dei Beni culturali- Società Chimica Italiana, 14-18 June, 2015, Bergamo, Italy
- 2) "Photocatalytic degradation of natural waxes deposit on artistic surfaces by means of TiO₂ nanoparticles" – GIULIA TORRIELLI, V.Caratto, F.Locardi, E.Sanguineti, L.Gaggero, M.Ferretti. XI NATIONAL CONFERENCE ON NANOPHASE MATERIALS, 26-28 October, 2015, Rome, Italy.
- 3) G. Torrielli, V. Caratto, L. Gaggero, M. Ferretti. *Innovative method and apparatus for deep cleaning of soluble salts from mortars and lithic materials*. European Geosciences Union, Wien 17-22 April 2016.
- 4) G.Torrielli, V. Caratto, L. Gaggero, M. Ferretti. *Innovative method for the cleaning of soluble salts from mortars and lithic materials*. Journées Franco-Italiennes de Chimie, Avignon 25-26 April 2016.
- 5) G. Torrielli, A.Provino, M.Ferretti, P.Manfrinetti. *Instrumental characterization of gypsum from the Monteverde's sculptures*. Conference *Scientia ad Artem*, Florence 8 June 2017.
- 6) G.Torrielli, G.Paolicelli, F.Locardi, M.Ferretti, G.Petrillo, *Oli siccativi: approccio multi-analitico per l'identificazione di finger-print*. Conference *Scientia ad Artem*, Florence 8 June 2017.
- 7) G.Torrielli, V.Caratto, S.Alberti, F.Fossati, M.Ferretti, *Nuovo metodo per la pulitura di affreschi da sali solubili*. Congresso Nazionale Società Chimica Italiana, Paestum 16-20 September 2017.
- 8) G.Torrielli, G.Paolicelli, F.Locardi, M.Ferretti, G.Petrillo. *Oli siccativi: approccio multi-analitico per l'identificazione di finger-print su campioni non trattati*. Congresso Nazionale Società Chimica Italiana, Paestum 16-20 September 2017.
- 9) G. Torrielli, A.Provino, M.Ferretti, P.Manfrinetti. *Idealità e Materialismo, caratterizzazione strumentale dei gessi di Giulio Monteverde*. Bistagno, (AL), 8 July 2017.

Congresses Attended

1. XV Congresso Nazionale Divisione di Chimica dell'Ambiente e Chimica dei Beni culturali- Società Chimica Italiana, June 14-18, 2015, Bergamo, Italy.
2. XI NATIONAL CONFERENCE ON NANOPHASE MATERIALS, October 26-28, 2015, Roma, Italy.
3. SICH-Prin, Sustainability in Cultural Heritage, Rome 11-12 January 2016.
4. IWIW, International workshop industrial waste, Genoa 17 February 2016.
5. EGU, European Geosciences Union, Wien 17-22 April 2016.
6. JFI, Journées Franco-Italiennes de Chimie, Avignon 25-26 April 2016.
7. XVI Congresso Nazionale della Chimica dell'Ambiente e dei Beni Culturali, Lecce 26-29 June 2016.
8. I jornada de Escultura Liger, Valencia (Spain), 24-25 March 2017.
9. La protezione dei beni culturali in area di crisi, Reggio Emilia, 10 September 2016.
10. Nanomateriales y Medio Ambiente, Zaragoza (Spain), 25-26 April, 2-3 May 2017.
11. Gipsoteche in penombra. Il percorso del fare, Gipsoteca G. Monteverde, Bistagno (AL), 8 July 2017.
12. XXVI Congresso Nazionale della Società Chimica Italiana. Paestum (SA) 10-14 September 2017.

Courseware

Courses attended

- Analisi multivariate dei dati, Prof. S.Lanteri, C. Armanino, R. Leardi (3 credits)
- Applicazione della Spettroscopia Raman ai materiali Prof. M. Carnasciali (2 credits)
- Fondamenti di Microscopia a scansione elettronica SEM/TEM (3 credits) - Course Given by Prof. P.Riani
- Nanocompositi polimerici- Prof. Orietta Monticelli
- Fondamenti e applicazioni del Metodo Rietveld- Prof. C. Artini

Courses given by invited experts:

- 1) "X-ray experimental techniques"- Morgante (31/03/2015)
- 2) "Yb and Eu correlated electron system"- (21-22/04/2015)
- 3) "Elementi di chimica forense"- Narizzano (18-19/05/2015)
- 4) Diagnostica multispettrale applicata ai beni culturali: dalle tecniche di base agli sviluppi computazionali. Dr. P. Triolo, Genoa 14 December 2016.
- 5) NIR Spectroscopy. Theory and application. Dr. T. Cattaneo, R. Giangiacomo, Genoa 29 Febbraio 2016.

National and International Schools or Workshops

- IV Scuola Nazionale di Chimica dell'Ambiente e dei Beni Culturali, July 13-16, 2015, Fisciano (SA).
- II Scuola Internazionale IPERION CH.it Training Camp 2015, October 15-20, 2015, Aquila (AQ).
- Colore & Conservazione, Milan 13-14 November 2015.
- Pulitura Laser per i Beni culturali, Dr. Brunetto 3-4 May 2016.
- Workshop: Autoproduzione di colori da ritocco: colori a Laropal A81 e acquerelli. Bergamo 2-3 December 2016
- Workshop sull'uso dell'Aquazol nelle operazioni di restauro delle opere policrome mobili. Reggio Emilia 20 January 2017.
- La ceramica della Sardegna Meridionale. Questioni aperte e nuove prospettive, Genoa 31 May-1 June 2017.
- Scientia ad Artem. Florence 8 June 2017.

Seminars Given

- 1) I Beni della Cappella di San Bernardo nella contrada di Saquana"- Un pellegrinaggio tra arte e cultura. Cartosio (AL), 04 July 2015.
- 2) Il restauro delle sculture lignee, "Giornate Fai di Primavera", Carpeneto (AL), 19-20 March 2016.
- 3) Risanare gli strappi dei dipinti su tela mediante polimeri sintetici. Acqui T., June 2017.
- 4) L'iconografia di San Rocco: simboli e caratteristiche. Bandita di Cassinelle (AL), July 2017.
- 5) Il San Rocco di Bandita: il restauro nel mondo contemporaneo. Bandita di Cassinelle (AL), August 2017.

Seminars Attended

- 1) Partecipazione al Seminario "Tensionamento e telai dei dipinti su tela tra tradizione ed innovazione"- (30-31/01/2015)-Piazzola sul Brenta (PD)
- 2) "The band between paper fibers"- Schennach (17/02/2015)
- 3) "Presentazione Assegni di Ricerca Po Cro FESR Liguria 2007-2013 Asse IV "Capitale Umano"- (19/02/2015)
- 4) L'impatto delle mie pubblicazioni scientifiche. Come pubblicare con successo sulle riviste scientifiche più importanti a livello internazionale, Dr. A. Newman 27 October 2015.
- 5) Design of magnetic nano-architecture, Dr. D. Peddis 22 April 2016.
- 6) Il restauro nell'era della fabbricazione digitale, Cesmar7, Archeolab, Parma 5 novembre 2016.
- 7) Arte e scienza: le scienze per i beni culturali- Torino 3 December 2016.
- 8) Le cave di pietra dell'antico Egitto- Prof A. Borghi, Genoa 11 January 2017.
- 9) L'alabastro di Busca tra arte e scienza, Prof A.Marengo, Genoa 11 January 2017.
- 10) Metodo layer-by-layer di preparazione di sistemi nanostrutturati, Prof.F. Carosio, Genoa 27 January 2017.
- 11) Usos artísticos del alabastro y procedencia del material, Zaragoza (Spain) 4 April 2017.

- 12) Nanomateriales como contaminantes emergentes, Dr. J.R. Castillo, Zaragoza (Spain) 25 April 2017.
- 13) Tecnicas de separacion, caracterizacion, deteccion y cuantificacion de nanomateriales, Dr. J Perez-Arantegui, Zaragoza (Spain), 2 May 2017.
- 14) Seguimiento de procesos de degradacion de nanoparticulas mediante metodo magneticos, Dr. L. Gutiérrez, Zaragoza (Spain), 3 May 2017.
- 15) Analisi termica associate al gas-massa. Dr. F. Locardi, Genoa 13 June 2017.

OtherActivities

- 1) Partecipazione corso "*In the mood for Mud*" - Museo diffuso Valli Bormida (22/05-10/07/2015)- Museo G. Monteverde, Bistagno (AL).
- 2) Supporto alla didattica come assistente di Laboratorio per il Corso di "Metodologie chimico-fisiche per i Beni Culturali" (2015-2016) della Laurea triennale in Conservazione dei Beni Culturali (Prof.G.Costa) avendo ottenuto il Riconoscimento di Cultore della materia per detto Corso.
- 3) Progettazione e organizzazione Laboratorio Festival della Scienza 2016, "*Panta Rei, Un Mare di Segni*" in collaborazione con Museo del Mare, Genoa.
- 4) Collaborazione e nomina di referente per la Liguria del ponente dell'A.I.A.M - Associazione per la valorizzazione e promozione di Mulini storici.
- 1) Assistenza Laboratorio Chimica-Fisica 1, Prof. M. Carnasciali.
- 2) Supporto alla didattica come assistente di Laboratorio per il Corso di "Metodologie chimico-fisiche per i Beni Culturali" (2016-2017 e 2017-2018) della Laurea triennale in Conservazione dei Beni Culturali (Prof.G.Costa) avendo ottenuto il Riconoscimento di Cultore della materia per detto Corso.
- 3) Guida museale volontaria presso Gipsoteca G. Monteverde, Bistagno, AL.
- 4) Collaborazione con restauratori del Basso Piemonte per studio diagnostico sui materiali componenti le opere d'arte.

ACTIVITY REPORT

Scientific Publications

[1] P. Piccardo, **J. Vernet**, G. Ghiara, Mise en oeuvre des alliages cuivreux, Comprendre et faire parler le métal grâce à la science des matériaux. In M.Pernot (eds) Quatre mille ans d'histoire du cuivre, 2017, p. 41-60.

[2] V. Bongiorno, **J. Vernet**, P. Piccardo, La statuaire funéraire contemporaine du Cimetière Monumental de Staglieno de Gênes, Italie. In M.Pernot (eds.) Quatre mille ans d'histoire du cuivre, 2017, p. 299-317.

[3] L. Sforzini, P. Piccardo, V. Bongiorno, **J. Vernet**, D. Fodaro, A. Lo Monaco, P. Martini, E. Franceschini, C. Pelosi, Doria Repository: New data and technical details in the light of the actual conservation project. In Proceedings Book 8th European Symposium on Religious Art Restoration & Conservation (ESRARC), eds. C. Pelosi, G. Agresti, L. Lanteri, C. Parisi, Viterbo (IT) 26-28th may 2016, pp. 139.

[4] M.Mödlinger, **J.Vernet**, Appendici: Analisi metallografiche dell'elmo e schiniere. In F.M. Gambari, B. Grassi, M.G. Ruggiero, Nuovi dati sul ripostiglio della Malpensa, *ZiXu Studi sulla cultura celtica di Golasecca*, Vol. II, pp. 161 – 196 (in press).

[5] **J.Vernet**, G.Ghiara, C.Risso, P.Piccardo, G.Voland, Recovering the casting process of ancient bronzes with SEM analysis: Metallographic investigations of Bronze Age as-cast bronzes and experimental casting ingots, *Microscopie*, Anno XIV – n°1 (27), 2017, p. 65,

[6] P. Piccardo, G. Ghiara, V. Bongiorno, **J. Vernet**, R. Spotorno. SEM on metal archaeological findings: case studies, *Microscopie*, Anno XIV – n°1 (27), pp. 59 – 61,

Communications at Conferences

Oral communications

[1] **J. Vernet**, P. Piccardo, Impact of the mould material on the as-cast artefact's microstructure, MeTools 2016: The metalworker and his tools: symbolism, function and technology in the Bronze and Iron Ages, 23-26 / 07 / 2016, Belfast (RU)

[2] **J. Vernet**, P. Piccardo, R. Leardi, L. Montesano, A. Pola, Colabilità e caratteristiche microstrutturali delle leghe Cu-Pb-Sn: indagare l'influenza combinata della composizione e dei parametri sperimentali con un approccio chemiometrico. 36° Convegno Nazionale dell'AIM, 21-22-23/09/2016, Parma (PR)

Poster Communications

[1] V. Bongiorno, **J. Vernet**, P. Piccardo. Characterization of the Angel of the Calcagno tomb from the Staglieno Monumental Cemetery, Genoa: alloy and natural and 'artistic' patinas. *Métal à Ciel Ouvert*, 4-6 /12/2014, Paris (FR).

[2] **J.Vernet**, V. Bongiorno, G. Ghiara, P. Piccardo. Multi-technical approach for the study of archaeological and artistic bronze objects. *InArt, 2nd International Conference on Innovation in Art Research and Technology*, 21-25/03/2016, Ghent (BE)

[3] **J. Vernet**, P. Piccardo, Role of lead as a major alloying element in tin bronzes of archaeological and artistic interest. *InArt, 2nd International Conference on Innovation in Art Research and Technology*, 21-25/03/2016, Ghent (BE)

[4] L. Sforzini, P. Piccardo, V. Bongiorno, **J. Vernet**, D. Fodaro, A. Lo Monaco, P. Martini, E. Franceschini, C. Pelosi, Doria Repository: New data and technical details in the light of the actual conservation project. *8th European Symposium on Religious Art Restoration & Conservation (ESRARC)*, 26-28th may 2016, Viterbo (IT).

[5] **J.Vernet**, G.Ghiara, C.Risso, G.Voland. Recovering the casting process of ancient bronzes with SEM analysis: Metallographic investigations of Bronze Age as-cast bronzes and experimental casting ingots. *Workshop teorico-pratico: La microscopia elettronica applicata allo studio dei Beni Culturali*, 06-07/02/2017, Urbino, PU (IT)

[6] **J. Vernet**, P. Piccardo. Out-of-Equilibrium Casting of Copper-based Alloys, Workshop PhD Program Federchimica, 24/05/2017, Genova (GE).

[7] **J. Vernet**, V. Bongiorno, G. Ghiara, C. Risso, P. Piccardo. Investigating Metallic Artefacts of Archaeological and Artistic Interest: Case Studies. SCIENTIA AD ARTEM 3 Workshop, 08/06/2017, Firenze (FI).

[8] **J. Vernet**, C. Bo, D. Maccio', P. Piccardo. Investigating the impact of cooling rate on the peritectic solidification of binary tin bronzes with DTA, MEDICTA 13th, 24-27/09/2017, Loano (SV). Premiato

Congresses Attended

[1] Métal à Ciel Ouvert,
04-06 / 12 / 2014, Paris (FR).

[2] InArt, 2nd International Conference on Innovation in Art Research and Technology
21-25 / 03 / 2016, Ghent (BE)

[3] MeTools 2016: The metalworker and his tools: symbolism, function and technology in the Bronze and Iron Ages, 23-26 / 07 / 2016, Belfast (RU)

[4] 36° Convegno Nazionale AIM
21-23 / 09 / 2016, Parma, PR (IT)

[5] MEDICTA 13th,
24-27/09/2017, Loano (SV).

COURSEWARE

Courses attended and passed (11 credits)

Courses – Type A (2 – 5 CFU requested)

Elementi di Chimica Forense (1CFU)

Dott. Narizzano Riccardo (ARPAL, Genova)

18/05 – 19/05/2015, DCCI (4 ore)

New methods for food authenticity and safety testing, (1CFU)

Dr.ssa V. Merlo (Technical Manager & Director, Eurofins, Cuneo)

27/11/2015, DCCI (4 ore)

Low and very low temperature, methods of producing / measuring cryogenic temperature (1CFU)

Ivan Curlik (University of Presov, Slovacchia)

17/02 – 19/02/2016, DCCI, (4 ore)

Advanced Materials for Renewable Energy (1CFU)

Prof. Peter Rogl (Institute of Physical Chemistry, University of Vienna, Autriche)

14 and 16/06/2016, DCCI (4 ore)

Part 1: Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials

Part 2: Novel Materials for Energy Storage and Conversion (1CFU)

Prof. Thomas Fässler (Technical University of Munich, Germany)

11/05/2016, DCCI (4 ore)

Courses – Type B (6 – 14 CFU requested)

Analisi multivariate dei dati chimici, 3CFU, (2015)

Verifica superata il 17/10/2017

Applicazione della spettroscopia Raman ai materiali, 2CFU, (2015)

Verifica superata il 24/12/2015

Metodi Matematici per la Chimica, 2CFU, (2015)

Senza verifica

Metodologia della ricerca sperimentale, Experimental Design, 3 CFU, (2016)

Verifica superata il 18/05/2016

Principi di metallurgia applicata: tradizione e innovazione, 2 CFU, (2016)

Verifica non superata

Sintesi, struttura e proprietà funzionali di composti intermetallici, 2CFU, (2016)

Verifica superata il 06/10/2017

Courses – Type F

Metallurgia I (Prof. P. Piccardo), 2014/2015

Corso Triennale di Chimica / Scienza dei Materiali

Metallurgia II (Prof. P. Piccardo), 2014/2015

Corso Magistrale di Chimica / Scienza dei Materiali

National and International Schools or Workshops

[1] Metallurgy Summer School. Experimental techniques for metal analysis: theory and applications organized by AIM and COMET, 26-29/07/2016, Bertinoro (FC) 5 CFU.

[2] Workshop teorico-pratico: La microscopia elettronica applicata allo studio dei Beni Culturali, 06-07 Febbraio 2017, Urbino, PU (IT).

[3] Summer School "Archeologia e beni culturali di terra e di mare. La pratica dello scavo archeologico e le nuove tecnologie di studio, documentazione ed esibizione"; Università degli Studi Suor Orsola Benincasa, 10-24 Settembre 2017, Procida (NA), 100 ore.

Seminars Attended

Giornata conclusiva, Assegni di Ricerca Po Cro FESR Liguria 2007-2013 Asse IV "Capitale Umano"

Seminario tenuto dagli assegnisti del DCCI, 19/02/2015

Electrochemical Impedance Spectroscopy – a tool for "in situ" investigation of SOFC anodes,

Dott.ssa G. Raikova. 22/09/2015, DCCI

Terzo anno di dottorato, XXVIII Ciclo, 5/11/2015, DCCI

- BAZZANO ANDREA, "Strumentazione di chimica analitica per l'esplorazione del sistema solare"
- GARBARINO SILVIA, "The magic of diazomethane: advantages and drawbacks of an elusive reagent"
- GHIARA GIORGIA, "Introduzione alle pile a combustibile e ai fenomeni di degrado ad alta temperatura"

Uso della tecnica laser nell'ambito della conservazione e del restauro dei Beni Culturali

Dott.ssa A. Brunetto. 04/05/2016, DCCI

Aspetti e prospettive della moderna industria siderurgica,
Ing. Franco Belgrano. 5/05/2016, DCCI

Didactical support

Course support

Metallurgia I (Prof. P. Piccardo), Corso Laurea Triennale di Chimica / Scienza dei Materiali / Beni Culturali

- liste

Metallurgia II (Prof. P. Piccardo), Corso Magistrale di Chimica / Scienza dei Materiali

“From the Stone to Metals: the beginnings of metallurgy”, (2 ore) with PhD M.Mödlinger

“First results on arsenical copper annealing”, (4 ore) with PhD M.Mödlinger

Bases de métallurgie et archéoméallurgie (Prof. P. Piccardo), Cours Master du Patrimoine Culturel & Archéométrie, Université Michel de Montaigne Bordeaux III, Francia

“Casting Techniques”, (2 ore)

Laboratorio Metallurgia per Beni Culturali (Prof. P. Piccardo), Corso Magistrale,
(6 ore) with PhD V. Bongiorno, Ph.D G. Ghiara

Thesis support

Margherita BIONDI, Laurea Triennale in Scienza dei Materiali, July 2015

“Leghe a base rame: contributo della Scienza dei Materiali alla messa a punto di test applicabili in archeologia sperimentale.”

Caterina BO, Laurea Triennale in Scienze e Tecnologie Chimiche, March 2017

“Impatto dei diversi materiali di stampi sulle caratteristiche microstrutturali delle leghe di rame di fonderia”

Chiara RISSO, Laurea Magistrale in Metodologie per la Conservazione e il Restauro dei Beni Culturali,
March 2017

“Metodologie per l'autenticazione di artefact archeologici e la detezone di falsi”

Mila CRIPPA, Laurea Magistrale in Metodologie per la Conservazione e il Restauro dei Beni Culturali,
June 2017. *“Caratterizzazione delle patine artistiche nella scultura contemporanea in metallo: produzione e conservazione nelle opere di Nedo Canuti”*

Other Activities

Avril 2017

Partecipazione allo studio e alla caratterizzazione di un reperto metallico di asce-lingotto proveniente di diversi depositi di Bourgogne Franche-Comté, Francia, CCE Lons-le-Saunier (FR)

Giugno 2016

I metalli oggi e nel futuro, esposizione al Festival dell'Università, Piazza Matteotti, 18-19/06/2016. Presentazione delle stampante 3D, pile a combustibile, metalli di fonderia.

Maggio 2016

Partecipazione allo studio e alla caratterizzazione di un reperto metallico di asce-lingotto proveniente di Loyette. DRAC Auvergne – Rhone Alpes, Lyon (FR)

Luglio 2015

Organizzazione di un workshop (3 giorni) in collaborazione con l'Université de Bordeaux III Michel Montaigne (Fr), per gli studenti della laurea magistrale Matériaux du Patrimoine Culturel & Archéométrie. *“Découverte des techniques métallographiques en laboratoire pour applications archéométriques”*

Luglio 2015

Partecipazione allo studio e la caratterizzazione di un elmo e schiniere dell'Età del Bronzo, ritrovati sul sito di Milano Malpensa, Soprintendenza Archeologica della Lombardia

Marzo 2015

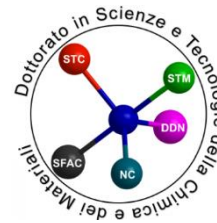
Partecipazione allo studio di un mausoleo (Tomba Fracchia) localizzato a Bargone: studio metallografico delle lastre di alluminio in vista di future operazione di restauro. In collaborazione con studentesse dell'Università d'Architettura, Genova, e restauratrice di ARTEMIS, Genova.

Luglio 2014 – Gennaio 2015

Analisi e caratterizzazione di reperti metallici archeologici della Liguria dell'Età del Bronzo e dell'Età del Ferro, Soprintendenza per i beni culturali e paesaggistici della Liguria.



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



Curriculum: Scienze e tecnologie chimiche

Silvia Villa

Start of the Doctorate Program November 1st, 2014

End of the Doctorate Program October 31st, 2017

Advisors

Prof. Fabio Canepa

Thesis Title

Magnetic nanoparticles for advanced applications

Thesis abstract

The research project mainly deals with the synthesis of magnetic nanoparticles, in particular superparamagnetic nanoparticles, and their application as nanoprobes in biomedical and analytical applications.

The main activities are carried out in the biomedical field, to create a magnetic nanocarrier to deliver drugs to a target and to study the subsequent drug release efficiency.

The high magnetic properties and the possible functionalizations of the synthesized nanoparticles are also optimal for the separation and removal of toxic metal ions from artificially polluted waters.

ACTIVITY REPORT

Research Activity

Research period abroad

From 15 August 2016 to 7 December 2016 at Norwegian University of Science and Technology (NTNU) in Trondheim (NO) I worked in the Nanolab facility at Department of Materials Science and Engineering; Supervisor: Gurvinder Singh.

Scientific Publications

Original publications on ISI Journals:

- 1) "Design and optimization of lipid-modified poly-(amidoamine) dendrimer coated iron oxide nanoparticles as probes for biomedical applications" A. Boni, G. Bardi, A. Bertero, V. Cappello, M. Emdin, A. Flori, M. Gemmi, C. Innocenti, L. Menichetti, C. Sangregorio, S. Villa and V. Piazza, *RSC Nanoscale*, 7, 7307, **2015**
- 2) "Different sol-gel preparations of iron-doped TiO₂ nanoparticles: characterization, photocatalytic activity and cytotoxicity" V. Caratto, F. Locardi, S. Alberti, S. Villa, E. Sanguineti, A. Martinelli, T. Balbi, L. Canesi, M. Ferretti, *J. Sol-Gel Sci. Technol.*, 1-8, **2016**
- 3) "Enhancement of TiO₂ NPs Activity by Fe₃O₄ 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 and M. Ferretti, *Materials* **2016**, 9, 771

- 4) "Functionalization of Fe₃O₄ NPs by Silanization: Use of Amine (APTES) and Thiol (MPTMS) Silanes and Their Physical Characterization" S. Villa, P. Riani, F. Locardi and F. Canepa. *Materials* **2016**, 9, 826
- 5) "Photocatalytic Fe-doped n-TiO₂: from synthesis to utilization of in vitro cell models for screening human and environmental nanosafety", T. Balbi, V. Caratto, R. Fabbri, G. Camisassi, S. Villa and M. Ferretti. *Resource-Efficient Technologies 0 0 0*, **2017**, 1–8
- 6) "Delivery Nanoplatforms Based on Sorafenib and Superparamagnetic Iron Oxide Nanoparticles for Magnetically Targeted Therapy of Hepatocellular Carcinoma" N. Depalo, R. M. Iacobazzi, G. Valente, I. Arduino, S. Villa, F. Canepa, V. Laquintana, E. Fanizza, M. Striccoli, A. Cutrignelli, A. Lopodota, P. Porcelli, A. Azzariti, M. Franco, M. L. Curri and N. Denora. *Nano Research* **2017**, 10 (7): 2431–2448
- 7) "Thiol functionalized magnetic nanoparticles for static and dynamic removal of Pb (II) ions from waters" S. Villa, P. Riani, F. Soggia, E. Magi and F. Canepa. Submitted to *International Journal of Environmental Science and Technology* (June 2017)
- 8) "Systematic study on TiO₂ crystallization via hydrothermal synthesis in the presence of different ferrite nanoparticles as nucleation seeds" S. Alberti, V. Caratto, S. Villa, G. Singh, A. Martinelli, M. Ferretti and F. Canepa. Accepted *Journal of Nanoscience and Nanotechnology* (September 2017)
- 9) "Structural effect of copper and nitrogen doping in TiO₂ for photocatalytic activity evaluation" A. Martinelli, S. Alberti, V. Caratto, F. Locardi, G. Pampararo, S. Villa, M. Ferretti. Submitted to *Journal of Solid State Chemistry* (October 2017)
- 10) "Studies on the Enzymatically Promoted Release of Organic Molecules Linked to Magnetic Nanoparticles" C. Lambruschini, S. Villa, L. Banfi, F. Morana, F. Silveti, P. Riani, R. Riva, A. Relini, F. Canepa. Submitted to *Chemistry European Journal* (October 2017).
- 11) "Ligand-exchange in thiol-functionalized gold nanoparticles investigated through thermogravimetric and evolved gases analyses" F. Locardi, E. Canepa, S. Villa, I. Nelli, M. Ferretti, F. Canepa. In preparation, to be submitted to *Journal of analytical and applied pyrolysis*.

Communications at Conferences

Oral communications:

- 1) XLIII Congresso Nazionale della Divisione di Chimica Inorganica della Società Chimica Italiana, Camerino 9-12 September 2015, "Capture of heavy metals metals by thiol functionalized magnetic nanoparticles using a system of permanent magnets" Silvia Villa, Paola Riani, Emanuele Magi, Fabio Canepa
- 2) Nanomedicine, Viterbo 21-23 September 2016. "Promising applications of magnetic multifunctional nanoparticles in biomedicine" S. Villa, C. Lambruschini, L. Banfi, P. Riani, F. Canepa, A. Relini, F. Morana, F. Silveti and R. Riva
- 3) 5th International Conference of Nanoscience and Materials Science. "Biocompatible multifunctional magnetic nanoparticles for possible applications in nanomedicine" S. Villa, L. Banfi, F. Canepa, C. Lambruschini, F. Morana, A. Relini, P. Riani, R. Riva, F. Silveti. Dubai 16-18 October 2017
- 4) World Congress on Nano Science and Nano Technology. "Biocompatible magnetic nanoparticles for possible applications in nanomedicine" S. Villa, L. Banfi, F. Canepa, C. Lambruschini, F. Morana, A. Relini, P. Riani, R. Riva, F. Silveti. Dubai 16-17 October 2017

Poster Communications:

- 1) "Structural and magnetic characterization of Co-carbides particles" S. Villa, P. Riani, F. Canepa CALPHAD XLIV, Loano 31 May – 5 June 2015
- 2) "Synthesis and characterization of Co-carbides particles" P. Riani, S. Villa, F. Canepa. XLIII Congresso Nazionale della Divisione di Chimica Inorganica della Società Chimica Italiana, 9-12 September 2015, Camerino
- 3) "Superparamagnetic Iron Oxide Nanocrystal and Sorafenib loaded PEG-terminated Micelles for Targeted Hepatic Carcinoma Therapy" N. Denora, N. Depalo, G. Valente, F. Canepa, S. Villa, V. Laquintana, E. Fanizza, M. Striccoli, M. L. Curri, A. Cutrignelli, A. Lopodota, M. Franco, presented among the project Nanomed, III Meeting, 23-24 April 2015, Bologna

- 4) "Superparamagnetic Nanoparticles and Sorafenib containing phospholipid micelles for targeted hepatic carcinoma therapy" BioMet15, XV Workshop on PharmacoBloMetallics 23-24 October 2015, Bari
- 5) "Magnetic Nanoparticles for biosensors, catalysts and high density permanent magnets" S. Villa, P. Riani, S. Fiorito, F. Canepa. NanotechITALY, Bologna 25-27 November 2015
- 6) "SPIONs/Sorafenib/micelles for magnetic drug delivery" S. Villa, F. Canepa, N. Denora, N. Depalo, School of Nanomedicine, Bari 2-4 December 2015
- 7) "The effect of the precursor on the synthesis and magnetic properties of Co and Co carbides NPs" S. Villa, P. Riani et F. Canepa, 20th International Conference on Solid Compounds of Transition Elements" SCTE-2016, Zaragoza, 11-15 April 2016
- 8) "The effect of the precursor on the synthesis and magnetic properties of Co and Co carbides NPs" S. Villa, P. Riani et F. Canepa, Journées Franco-Italiennes de Chimie, Avignone, 25-26 April 2016
- 9) "Synthesis, characterization and photocatalytic activity of Fe₃O₄-TiO₂ nanopowders" S. Villa, V. Caratto, F. Locardi, F. Canepa et M. Ferretti. Journées Franco-Italiennes de Chimie, Avignone, 25-26 April 2016
- 10) "Multifunctional fluorescent magnetic nanoparticles for potential biomedical applications" S. Villa, C. Lambruschini, R. Riva, L. Banfi, P. Riani, A. Relini and F. Canepa, Journées Franco-Italiennes de Chimie, Avignone, 25-26 April 2016
- 11) "Design and Synthesis of Multifunctional Fluorescent Magnetic Nanoparticles for Promising Biomedical Applications" C. Lambruschini, S. Villa, L. Banfi, F. Canepa, F. Morana, A. Relini, P. Riani, R. Riva and F. Silveti. XII Congresso del Gruppo Interdivisionale di Chimica Organometallica della Società Chimica Italiana Genova, 5 - 8 June 2016
- 12) "New synthesis of Fe₃O₄-TiO₂ nanopowders for removal of organic pollutants in water" S. Villa, V. Caratto, F. Locardi, S. Alberti, M. Sturini, A. Speltini, F. Maraschi, F. Canepa et M. Ferretti. XVI CONGRESSO NAZIONALE DI CHIMICA DELL'AMBIENTE E DEI BENI CULTURALI Lecce, 26-29 June 2016
- 13) "Investigation of functionalized nanoparticles through DTA/TGA – GC/MS coupling" F. Locardi, I. Nelli, S. Villa, F. Canepa, V. Caratto, M. Ferretti, G. A. Costa. AICAT 2016 XXXVIII National Congress on Calorimetry, Thermal Analysis and Applied Thermodynamics, Ischia 25-28 September 2016
- 14) "Capture and recovery of heavy metals through functionalized magnetic NPs" S. Villa, P. Riani, E. Magi, F. Canepa. Nano@NTNU Symposium 2016, Trondheim 17-18 November 2016
- 15) "Core/shell bi-magnetic nanoparticles: synthesis and magnetic properties" S. Villa, D. Peddis, G. Singh, F. Canepa. 24th International Symposium on Metastable, Amorphous and Nanostructured Materials – ISMANAM 2017, Donostia-San Sebastian, Spain 18-23 June 2017
- 16) "Synthesis and magnetic properties of multi-shell bi-magnetic nanoparticles" S. Villa, D. Peddis, G. Singh, F. Canepa. 5th Italian Conference on Magnetism – Magnet 2017, Assisi, 13-15 September 2017
- 17) "Functionalized nanoparticles investigated through thermal and evolved gas analyses" F. Locardi, I. Nelli, F. Palazon, V. Caratto, S. Villa, G. A. Costa, F. Canepa, M. Ferretti. 13th Mediterranean Conference on Calorimetry and Thermal Analysis - Medicta 2017, Loano, 24-27 September 2017
- 18) "Magnetically Targeted Delivery of Sorafenib to Liver Using Solid Lipid Nanoparticles for Treatment of Hepatocellular Carcinoma" N. Depalo, F. Vischio, I. Arduino, S. Villa, F. Canepa, E. Fanizza, B. Chul Lee, V. Laquintana, A. Lopodota, A. Cutrignelli, M. Principia Scavo, M. Striccoli, A. Agostiano, M. L. Curri, N. Denora. Applied Nanotechnology and Nanoscience International Conference – ANNIC 2017, Rome, 18-20 October 2017

Congresses Attended

- 1) CALPHAD XLIV Loano, 31 May – 5 June 2015
- 2) XLIII Congresso Nazionale della Divisione di Chimica Inorganica della Società Chimica Italiana, Camerino 9-12 September 2015

- 3) NanotechItaly, Bologna 25-27 November 2015
- 4) Journées Franco Italienne de Chimie, Avignone, 25-26 April 2016
- 5) Nanomedicine, Viterbo 21-23 September 2016
- 6) Nano@NTNU Symposium 2016, Trondheim 17-18 November 2016
- 7) 24th International Symposium on Metastable, Amorphous and Nanostructured Materials – ISMANAM 2017, Donostia-San Sebastian, Spain 18-23 June 2017
- 8) 5th International Conference of Nanoscience and Materials Science. Dubai 16-18 October 2017
- 9) World Congress on Nano Science and Nano Technology, Dubai 16-17 October 2017

Courseware

During the 3 years PhD course Silvia Villa has acquired 13 credits of Courseware.

Courses attended

Courses Given by Teachers of the DCCI:

- 1) Applicazione della spettroscopia Raman ai materiali, Prof. Marilena Carnasciali (2)
- 2) Materiali magnetici funzionali, Prof. Fabio Canepa (2)
- 3) Nanocompositi polimerici, Prof. Orietta Monticelli (2)
- 4) Soft Matter, Prof. Annalisa Relini DIFI (2)
- 5) Fondamenti di microscopia elettronica a scansione ed in trasmissione, Prof. Paola Riani (3)
- 6) Nanoparticle characterization by atomic force microscopy and dynamic light scattering, Prof. Ranieri Rolandi DIFI (2)

Courses Given by invited experts:

- 1) "X-ray experimental techniques" Prof. A. Morgante, CNR-IOM and Physics Department Trieste University, 31 March 2015
- 2) "Yb and Eu strongly correlated electron systems" Dr. Ivan Curlik, University of Presov Slovacchia, 21-22 April 2015
- 3) "Elementi di chimica forense" Dr. Narizzano, ARPAL 18-19 May 2015
- 4) "Modern Materials for Energy Saving (Renewable Energy)" Prof. Peter Rogl, University of Wien, 9-10 June 2015
- 5) "Magnetic Hyperthermia: from fundamentals to biomedical applications" Dr. Francisco Teràn 5-6 May 2016, IIT
- 6) "Synthesis, characterization and properties of intermetallic compounds and intermetallic clusters" Prof. Fassler 11 May 2017, DCCI

National and International Schools or Workshops

- 1) "Nuovi materiali ed energie sostenibili" Bressanone 13-16 July 2015.
- 2) School of Nanomedicine Bari 2-4 December 2015
- 3) IWIW 2016 - International Workshop on Industrial Waste, Genoa, Italy, 17 February 2016
- 4) Workshop "Nanostructured metal optics: from Theory to Enhanced Spectroscopies, Sensing, Imaging. Pisa, 1 April 2016
- 5) International symposium on Nanomedicine, Politecnico di Milano 31 May 2017

Seminars Attended

- 1) "The bond between paper fibers" Dr. Schennach, 17 February 2015 (DCCI)
- 2) "Recent cosmetic science and formulation technology" Y. Yamashita, 3 March 2015 (CNR-IENI)
- 3) "Design of magnetic nano-architecture" Dr. Davide Peddis 22 April 2016
- 4) "NIR Spectroscopy. Theory and application." 29 February 2016

- 5) Dott. Federico Carosio "Surface modification in a step by step manner: layer by layer assembly" 27 January 2017, DCCI (all'interno del corso di Nanocompositi polimerici)
- 6) Dott. A. Bianco (Istituto nazionale di astrofisica) "Sviluppo di nuovi materiali per olografia: dalla molecola al materiale";
Dott. A. Zanutta "Fotopolimeri in astronomia: aspetti pratici e risultati in cielo";
Dott. M. Landoni "Dal problema astronomico alla strumentazione: essere a metà tra scienza e tecnologia"
3 February 2017, DIFI
- 7) Prof. Sergio Riva (ICRM Milano) "Biocatalysis and natural products: a fruitful interaction" 12 June 2017 DCCI
- 8) Dott. Federico Locardi "Analisi termica accoppiata alla gascromatografia e spettrometria di massa. Un potente strumento per la caratterizzazione dei materiali" 13 June 2017, DCCI
- 9) Prof. J. K. Sello "Novel molecules and strategies for the treatment of infectious diseases" 3 July 2017, DCCI
- 10) Prof. Julian Sereni "Cryocooler materials for adiabatic demagnetization: comparison between paramagnetic salts and intermetallic compounds" 4 July 2017, DCCI
- 11) Dott. Paolo Mele "On research activities at Muroran Institute of Technology" 24 July 2017, DCCI

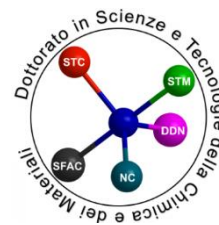
Other Activities

- 1) Participation in Organization & Management of CALPHAD XLIV, Loano 31 May – 5 June 2015
- 2) Proposal submitted in response to the Call Investigator Grant - IG 2016 AIRC "Magnetic nanovectors for local and site-specific drug delivery in hepatocellular carcinoma or liver dominant metastasis"
- 3) Tutor didattico per il corso di Chimica generale ed Inorganica tenuto dalla Prof. Zanicchi per il corso di laurea in Chimica e Tecnologie Chimiche e per il corso di Chimica generale ed Inorganica tenuto dalla Prof. Riani per il corso di laurea in Scienze dei materiali (A.a. 2015-2016).
- 4) Assistente al Laboratorio didattico del corso di Chimica Fisica 1 tenuto dalla Prof.ssa Carnasciali (A.a. 2015-2016).
- 5) Proposal submitted in response to the Call Investigator Grant - IG 2017 AIRC "Magnetic nanovectors for local and site-specific drug delivery in hepatocellular carcinoma or liver dominant metastasis"



Università degli Studi di Genova

Doctorate in Sciences and Technologies of Chemistry and Materials



Curriculum: Drug Discovery

Valentina Vozella

Start of the Doctorate Program: *November 1st, 2014*

End of the Doctorate Program: *October 31st, 2017*

Advisor: *Prof. Daniele Piomelli*

Co-Advisor: *Prof. Olga Bruno*

Thesis Title: Study of sphingolipid-mediated signaling and metabolism during aging.

Thesis abstract

Many age-related diseases such as dementia, memory impairment, cognitive dysfunction, Alzheimer's disease (AD) and Parkinson's disease (PD) are associated with alterations in sphingolipid metabolism, but little is known about their role in normal aging. Even less is known about cognitive aging and the role of sphingolipids in specific brain areas such as the hippocampus. Hippocampi from male and female mice (3, 12 and 21 months old) were analyzed and age and sex-dependent accumulation of ceramide, hexosylceramide and sphingomyelin were observed. In particular, an age-dependent accumulation of sphingolipids containing nervonic acid (24:1) was observed in 21 month-old male and female mice. The gender-biased difference in accumulation of sphingolipids in the hippocampus of old mice suggests that additional factors might be involved, for example menopause.

To further investigate the link between aging and ceramides, 84 healthy women and 80 healthy men, with age ranging from 25 to 82 years old, were recruited and ceramides were analyzed in plasma. Results indicate a strong gender-related difference in levels of ceramide 24:1. Compared to age-matched men, young women (21 to 40 year old) showed significantly lower plasma levels of ceramide 24:1. Indeed, while men did not show any significant age-related increase in ceramide 24:1, aging was associated with increased ceramide 24:1 levels in females and the highest increase was found to occur in the perimenopausal period (41-50 and 51-60 year old). This discovery suggested that hormonal changes occurring in this period may play a role. Subjects were divided in pre- and post-menopause and estradiol levels were found significantly decreased in post-menopause women, while Ceramide 24:1 plasma levels are significantly increased in post-menopause female subjects. Employing a Pearson's regression model we found that a strong negative correlation is present in healthy female subjects.

ACTIVITY REPORT

Research Activity

Research Period Abroad

The research activity was carried out at the IIT-Italian Institute of Technology, Drug Discovery and Development department for the 1st and 2nd year.

Valentina Vozella has spent a research period of 12 months abroad (her entire 3rd year), carrying out researches at the University of California Irvine (Irvine-USA) under the supervision of Prof. Daniele Piomelli and Prof. Kwang-Mook Jung, from 24th October 2016 to 31st October 2017.

Scientific Publications

1. **V. Vozella**, A. Basit, A. Misto, D. Piomelli. "Age-dependent changes in nervonic acid-containing sphingolipids in mouse hippocampus", DOI: 10.1016/j.bbalip.2017.08.008. *Biochimica et Biophysica Acta (BBA) - Molecular and Cell Biology of Lipids*, **2017**, 1862, pp. 1502-1511.
Impact factor: 5.557
2. A. Bach, D. Pizzirani, N. Realini, **V. Vozella**, D. Russo, I. Penna, L. Melzig, R. Scarpelli, D. Piomelli. "Benzoxazolone Carboxamides as Potent Acid Ceramidase Inhibitors: Synthesis and Structure-Activity Relationship (SAR) Studies", DOI: 10.1021/acs.jmedchem.5b01188. *J. Med. Chem.*, **2015**, 58, pp 9258-9272.
Impact factor: 6.259
3. A. Misto, A. Basit, G. Provensi, **V. Vozella**, M.B. Passani, D. Piomelli. "Mast cell-derived histamine controls liver ketogenesis via OEA signaling" (manuscript under review, *Cell Metabolism*)
Impact factor: 17.303
4. A. Basit, G. Spalletta, **V. Vozella**, N. Realini, A. Armirotti, S. Sensi, D. Piomelli. "Circulating ceramide levels correlate with premorbid brain structural damage in middle-life women" (manuscript in preparation)

Communications at Conferences

Poster Communications:

1. **V. Vozella**, N. Realini, A. Misto, D. Piomelli. "Feeding regulates sphingolipid-mediated signaling in mouse hypothalamus".
Poster presented at *Gordon Research Conference Lipids, molecular and cellular biology of* (Waterville Valley, New Hampshire, USA, July 30-August 4, **2017**)
2. **V. Vozella**, N. Realini, A. Misto, D. Piomelli. "Feeding regulates sphingolipid-mediated signaling in mouse hypothalamus".
Poster presented at *Keystone Symposia on Molecular and Cell Biology, Lipidomics and Bioactive Lipids in Metabolism and Disease* (Tahoe City, California, USA, February 26-March 2, **2017**)

3. **V. Vozella**, N. Realini, A. Misto, D. Piomelli. “Feeding regulates sphingolipid-mediated signaling in mouse hypothalamus”.
Poster presented at *Society for Neuroscience (SfN)* (San Diego, California, USA, 12-16 November **2016**)
4. **V. Vozella**, N. Realini, A. Misto, D. Piomelli “Feeding status regulates ceramide signaling in mouse hypothalamus”
Poster presented at *EMBO Workshop on Neural Control of Metabolism and Eating Behavior* (Cascais, Portugal, 5-7 May **2016**)

Congresses Attended

1. **Gordon Research Conference** - Lipids, molecular and cellular biology of, 30 July - 4 August **2017**, Waterville Valley, New Hampshire, USA
2. **Keystone Symposia** on Molecular and Cell Biology, Lipidomics and Bioactive Lipids in Metabolism and Disease, 26 February - 2 March **2017**, Tahoe City, California, USA
3. **SFN - Society For Neuroscience**, 12 - 16 November **2016**, San Diego, California, USA
4. Neural Control of Metabolism and Eating Behavior, **EMBO conference**, 5-7 May **2016**, Cascais, Portugal
5. Drugs of abuse and mental diseases, **1st Zardi Gori Foundation Conference**, 5-6 November **2015**, Milan, Italy
6. **7th European Workshop on Cannabinoid Research and IACM 8th Conference on Cannabinoids in Medicine**, 17-19 September **2015**, Sestri Levante, Italy

Courseware

Courses attended and passed (12 credits)

Courses Given by Teachers of the Unige and IIT:

Courses Given by Teachers of the DIFAR-UniGe:

- 1) Analisi multivariata dei dati chimici (3 credits)
- 2) Biotecnologie Farmaceutiche (3 credits)

Courses Given by Teachers of the Drug Discovery and Development department – IIT:

- 1) Target identification and validation (2 credits)
- 2) Hit identification (1 credit)
- 3) Hit to lead and lead optimization (3 credits)

Courses given by invited experts (3 credits)

- 1) New methods for food authenticity and safety testing. Dr.ssa Valeria Merlo *PhD, Direzione tecnica* – Technical Manager & Director, Eurofins, Cuneo. (1 credit)
- 2) X-ray based experimental techniques and characterization of nano-materials. Alberto Morgante, CNR-IOM and Physics Department, Trieste University. (1 credit)
- 3) Elementi di Chimica Forense. Dott. Narizzano Riccardo e Dott.ssa Risso Fulvia, ARPAL, Genova. (1 credit)

National and International Schools or Workshops

- 1) SoSMSE Summer School (School on Science Management for Scientists and Engineers)
2 weeks (11 - 22 July 2016), Genova, Italy.
- 2) Workshop: Genomics and Health
23 June 2016, IIT, Genova.
 - **Mediterranean Diet has Impact on Aging: The Role of Telomeres.** *Prof. Immacolata De Vivo, Harvard Medical School/Brigham and Women's Hospital*
 - **Protein-RNA interactions and function on alternative 3'UTRs.** *Prof. Christopher Burge, Massachusetts Institute of Technology*
- 3) Publishing Scientific Research; Trends, Impact Factors, Open Access, eBooks, Peer Review, and much more. Demonstration Springer free Tools, 2 October 2015, IIT, Genova

Seminars Attended (2 credits)

- 1) **Impacts of technology in economic terms.** *Dr Michael Spence, IIT-Genova, 16/12/2014*
- 2) **How Italian decree 26/2014 on animal welfare changes the use of animals for scientific or educational purposes.** *Dr.ssa Gemma Perretta, Cellular Biology and Neurobiology Institute (IBCN) National Research Council of Italy- Roma, IIT-Genova, 28/01/2015*
- 3) **Animal welfare: a human responsibility that encompasses all aspects of animal well-being.** *Dr.ssa Francesca Galbiati, Services Manager Italy, Charles River, IIT-Genova, 28/01/2015*
- 4) **Gene Editing: CRISPR/Cas9. The Scientific Basis and Advantages of the GE HealthCare Dharmacon System.** *Dr Peter Mahr, Gene Modulation Specialist -GE Healthcare – Dharmacon; Dr Johanna Decastroace, Scientific Support Scientist GE Healthcare – Dharmacon, IIT-Genova, 14/04/2015*
- 5) **Key Technologies for Pluripotent Stem Cells: Reprogramming Options, Culture Options, Stem Cell Characterization, Differentiation.** *Jerome Cabeau, Technical Sales Specialist, Life Sciences Solutions, Stem Cells, Drug Discovery & ADME/Tox Systems, IIT-Genova, 7/5/2015*
- 6) **Metabolomics Profile of Hypoxic Colorectal Cancer Cells (0.5 CFU).** *Dott. Alessandro Valli, Research Scientist presso il Weatherall Institute of Molecular Medicine, University of Oxford, Difar-sezione Chimica del farmaco e del Prodotto cosmetico, 8/5/2015*
- 7) **Hsp90 nella terapia antitumorale: dall'analisi conformazionale al disegno di nuovi inibitori allosterici (0.5 CFU).** *Dott. Gerolamo Vettoretti, Polo Alberti, 25/05/2015*
- 8) **Corticostratial Circuitry Control of Actions and Habit Learning.** *Dr. David Lovinger, Chief - National Institute on Alcohol Abuse and Alcoholism (National Institutes of Health - NIH) - Bethesda, MD – USA, IIT-Genova, 27/05/2015*
- 9) **Chemical biology of glycosphingolipid metabolism in man.** *Dr. Herman Overkleeft, Leiden Institute of Chemistry, IIT-Genova, 29/05/2015*
- 10) **Contribution of chemistry to sphingolipid research.** *Prof. Gemma Fabriàs, IIT-Genova, 3/07/2015*

- 11) **Modelli per lo studio in vitro del metabolismo umano.** *Arti Ahluwalia Professore Associato di Bioingegneria Industriale Dipartimento di Ingegneria dell'Informazione Università degli Studi di Pisa, Dipartimento di Medicina Sperimentale, 16/07/2015.*
- 12) **Antral oocytes: chromatin organization and embryo development.** *Drs. Manuela Monti, Centro di medicina rigenerativa, Fondazione IRCCS, Policlinico San Matteo, Pavia, IIT-Genova, 2/11/2015*
- 13) **The Challenge of Brain Disease.** *Prof. Colin Blakemore, Professor of Neuroscience and Philosophy, School of Advanced Study, University of London Emeritus Professor of Neuroscience, University of Oxford, IIT-Genova, 10/12/2015*
- 14) **Can we selectively turn on aberrantly methylated genes?** *Dr. Annalisa Di Ruscio, Instructor of Medicine at Harvard Medical School, Boston, USA; Resercher at Department of Translational Medicine, Eastern Piedmont University, Novara, Italy, IIT-Genova, 14/01/2016*
- 15) **Oxidative Stress in Aging and Human Diseases – Exploring the Mechanisms.** *Wei Cao, IIT-Genova, 22/02/2016*
- 16) **The transcription factor STAT3 at the crossroads between inflammation and cancer.** *Prof. Valeria Poli, Molecular Biotechnology Center, University of Turin, IIT-Genova, 11/05/2016*
- 17) **FGF signaling and surface area growth and gyrification of the neocortex.** *Prof.ssa Flora M. Vaccarino, Department of Neurobiology, Yale University School of Medicine, New Haven, Connecticut, IIT-Genova, 23/06/2016*
- 18) **The control of myogenesis: from coding to non-coding RNAs and back.** *Prof.ssa Irene Bozzoni Dept. of Biology and Biotechnology "Charles Darwin" Sapienza - University of Rome, IIT-Genova, 23/06/2016*
- 19) **Remodelling of brain circuitry in chronic pain.** *Prof. Marco Martina Northwestern University, Feinberg School of Medicine Chicago, IIT-Genova, 8/07/2016*
- 20) **Alpha-synuclein conformational states and their impact on vesicles trafficking.** *Prof. Luigi Bubacco, University of Padova, IIT-Genova, 7/09/2016*
- 21) **Using the human laboratory to investigate the analgesic effects and abuse liability of cannabis and cannabinoids.** *Dr. Ziva Cooper, Associate Professor of Clinical Neurobiology Department of Psychiatry Columbia University Medical Center, UCI-Irvine, 25/01/2017*
- 22) **Glutamate receptors drive the construction of a hippocampal feedforward inhibitory pathway.** *Dr. Chris McBain, Laboratory of Cellular and Synaptic Neurophysiology, National Institutes of Health (NIH), UCI-Irvine, 31/01/2017*
- 23) **The Habenulo-Interpeduncular Pathway: Nicotine Aversion and Beyond.** *Dr. Christie Fowler, Neurobiology & Behavior UC Irvine, UCI-Irvine, 13/02/2017*
- 24) **Understanding development of depression: choose your own adventure story.** *Prof. Benjamin L. Hankin, Psychology University of Illinois Urbana-Champaign, UCI-Irvine, 21/02/2017*
- 25) **Molecular Mechanisms of Memory Storage: Sleep, epigenetics and neurodevelopmental disorder.** *Professor Ted Abel, Molecular Physiology and Biophysics at Carver College of Medicine, University of Iowa, UCI-Irvine, 7/03/2017*
- 26) **Synaptic and epigenetic plasticity induced by early life experience drives life-long emotional and cognitive resilience.** *Tallie Z. Baram, Professor of Pediatrics, Anatomy & Neurobiology, Physiology & Biophysics, UCI-Irvine, 24/04/2017*
- 27) **Neural Stem and Progenitor Cells in Cerebral Cortex Development and Regeneration.** *Robert F. Hevner, Professor of Neurological Surgery and Pathology, University of Washington, UCI-Irvine, 22/05/2017*

Other Activities

- 1) Supervised Sophia Levis, M.D. /PhD Student - Medical Scientist Training Program at UC Irvine School of Medicine, June - August 2017.
- 2) Supervising Paoula Choobchian, undergraduate student – Bio199 at UC Irvine, September 2017 - present
- 3) Supervising Andalib Danandeh, M.D. – junior specialist at UC Irvine, September 2017 - present
- 4) Supervising Brandon Max McNeil, undergraduate student – Bio199 at UC Irvine, October 2017 - present



Università degli Studi di Genova

Doctorate School in

Sciences and Technologies of

Chemistry and Materials

Curriculum: Chemical Sciences and Technologies

Yao Wang

Start of the Doctorate Program *November 1st, 2014*

End of the Doctorate Program *October 31st, 2017*

Advisors

Prof. Gabriele Cacciamani

Thesis Title

Thermodynamic modeling of alloy systems related to Co-based superalloys and related metallic coatings

Thesis abstract

The project will investigate phase relations of Co-based systems with a focus on stability of some phases by experimental and theoretical methods. Aim of this project is twofold.

One side is to establish phase diagrams of some systems containing Co that can contribute to the design of new materials. The understanding of phase diagrams for alloy systems is extremely important because there is a strong correlation between phase equilibria, microstructure and properties. In addition, phase diagrams can provide valuable information about melting, casting, crystallization, and other phenomena.

The other side is to investigate phase stability of TCP phases (Laves, σ , etc.) in intermetallic systems. Compositions and features of phases play a decisive role in the performance of alloys: some of them have a positive influence, as in the case of the alloy strengthening effect of $L1_2$, others, such as Laves, sigma, etc., are detrimental.

ACTIVITY REPORT

Research Activity

Scientific Publications

Original publications on ISI Journals:

- 1) “Thermodynamic modeling of the Al-Cr-Ni system over the entire composition and temperature range” Yao Wang, Gabriele Cacciamani, J. Alloy. Compd. 688 (2016) 422-435.
- 2) “Thermodynamic modelling of a six component (C-Co-Cr-Ni-Ta-W) system for the simulation of Cobalt based alloys” Gabriele Cacciamani, Giacomo Roncallo, Yao Wang, Erica Vacchieri, Alessio Costa. J. Alloy. Compd. 730 (2018) 291-310.
- 3) Yao Wang , Gabriele Cacciamani. “Cobalt-Chromium-Nickel” and “Chromium-Nickel-Tungsten” accepted for the publication in the MSIT workshop.
- 4) Yao Wang, Gabriele Cacciamani. “Experiment investigation and thermodynamic assessment of the Al-Co-Ni system” submitted to “Materials & Design”

Communications at Conferences

Poster Communications:

- 1) Ir effect on phase stability of NiCoCrAlY coatings for gas turbine component application in the “XLIV International Conference on Computer Coupling of Phase Diagrams and Thermochemistry”, May 31-June 5, 2015, Loano(Italy)
- 2) Thermodynamic modeling of the Co-Cr-Ta system in “CALPHAD meeting XLVI International Conference on Computer Coupling of Phase Diagrams and Thermochemistry”, June 11 - 16, 2017,Saint-Malo (France)
- 3) Thermodynamic modeling of a Co based superalloy applied to the prediction of the fcc-hcp phase transformation in gas turbine components during service (G. Cacciamani, G. Roncallo, Y. Wang, A. Costa, E. Vacchieri) in “36° Convegno Nazionale AIM”, 21-23 Settembre 2016, Parma, Italy

Oral Communications:

- 1) Thermodynamic modeling of the Al-Cr-Ni system over the entire composition and temperature range (Yao Wang and Gabriele Cacciamani) in “Giornate Italo-Francesi di Chimica”, 25-26 Aprile 2016, Avignon, France.

Congresses Attended

- 1) XLIV International Conference on Computer Coupling of Phase Diagrams and Thermochemistry (May 31-June 5, 2015, Loano(Italy)
- 2) Giornate Italo-Francesi di Chimica, 25-26 Aprile 2016, Avignon, France.
- 3) XLVI International Conference on Computer Coupling of Phase Diagrams and Thermochemistry, June 11 - 16, 2017,Saint-Malo (France)

Courseware

Courses attended and passed (12 credits)

Courses Given by Teachers of the

- 1) Metodi Matematici per la Chimica Given by Prof. of G.Figari, M.Rui, V.Magnasco (2 credits)
- 2) Scienza delle Superfici (Surface Science) Given by Prof. of Luca Vattuone (3 credits)
- 3) Struttura elettronica nei solidi (Trattazione Elementare) Given by Prof. of L. Manna (3 credits)
- 4) Caratterizzazione di nanoparticelle per mezzo della microscopia a forza atomica e Dynamic Light Scattering Given by Prof. of R. Roland (2 credits)
- 5) Sintesi, struttura e proprietà funzionali di composti intermetallici Given by Prof. A.Saccone (2 credits)

Courses Given by invited experts:

- 1) X-ray based experimental techniques and characterization of nano-materials (Alberto Morgante – 31 Marzo 2015)
- 2) Yb and Eu correlated electron systems (Dr. Ivan Curlik - 21-22 Aprile 2015)
- 3) Modern Materials for Energy Saving (Renewable Energy) (Peter Rogl - 10 giugno 2015)
- 4) Medicinal chemistry with carbohydrates: the influenza virus and the discovery of sialidase inhibitors (Prof. Ssa Anna Bernardi – 13 Novembre 2015)
- 5) Superfici ed interfacce in sistemi metallo-ceramici (Dr. Alberto Passerone, 16 and 19 May, 2017, DCCI)
- 6) Superhard Materials: Structural chemistry of boron and borides (Prof. Peter Rogl, 6-7 June, 2017, DCCI)

National and International Schools or Workshops

- 1) 30th Annual MSIT Meeting, 31 Jan-5 Feb 2016, Ringberg Castle, Germany
- 2) 5th Workshop "Programma PhD: La formazione post lauream e il mondo del lavoro - Nell'Industria Chimica, chi fa Ricerca... fa Carriera?" Federchimica (Italian Association of Chemical industries), 24th November, 2016, Noble Hall of the Polytechnic School of Genoa University.
- 3) Advanced Workshop on High-Performance & High-Throughput Materials Simulations using QUANTUM ESPRESSO 16 - 27 January 2017, Trieste, Italy.
- 4) 31th Annual MSIT Meeting, 12 -17 March 2017, Ringberg Castle, Germany
- 5) School for Advanced Thermodynamic Assessments, 3 - 7 July 2017, Peninsula of Giens, France.

Seminars Given

- 1) "Ir effect on phase stability of NiCoCrAlY coatings for gas turbine component application" Oral presentation in Ansaldo company (30/7/2015)
- 2) "Al-Co-Cr-Ni-Y database" Oral presentation in Ansaldo company (20/7/2017)

Seminars Attended

- 1) Seeing molecules: A survey on Non-optical Microscopies and their Applications (Martinez Espinoza Maria Isabel – 6 Novembre 2015)
- 2) The hydrogen autotransfer process (Spallarossa Martina – 6 Novembre 2015)
- 3) Chemicophysical exchanges in TiC reinforced metal matrix composites (Dr. Olivier Dezellus – 20th Aprile 2017,CNR)
- 4) Atomic structure and mass-production of size selected nanoparticles (Richard E. Palmer – 30th May 2017, DIFI)

5) An overview of proximal optimization and its applications to data science (Patrick L. Combettes – 12th July 2017, iit)

6) On research activities of Muroran Institute of Technology (Paolo Mele – 24th July 2017, DCCI)

Other Activities

1) Contribution to the organisation of the CALPHAD XLIV international conference (Loano, 31/5-5/6/2015)

2) An assistant for the course “solid state inorganic chemistry” given by Prof. Cacciamani (2016) for the “Laurea Magistrale in Scienze Chimiche”



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



Curriculum: Scienze Farmaceutiche, Alimentari e
Cosmetologiche

MENGYING YAN

Start of the Doctorate Program *November 1st, 2014*

End of the Doctorate Program *October 31, 2017*

Advisors

Prof. Gabriele Caviglioli

Thesis Title

Development and characterization of scaffolds for 3D cell culture

Thesis abstract

In many chemical technological fields, including biocides, cosmetics, medical devices, phytochemicals, medicinal products, etc., efficacy and toxicity studies are required for pure substances and formulations. Health surveillance and regulatory agencies in many countries are urging for the development of alternative methods to replace experiments on animals in the aforementioned areas. Thus, experiments on cell cultures are developed and performed worldwide. Traditional methods of cell culture have been studied on 2-dimensional (2D) surfaces such as Petri dishes, tissue culture flasks, and micro-well plates, which have been shown to be insufficient for new challenges. Three-dimensional cell culture matrices, also known as scaffolds, were introduced to overcome 2D culture limitations. My study is focus on research and development of new matrix-scaffold with better performance for 3D cell culture, which can be applied in the cell biology and biochemistry, as well as pharmaceutical studies or in tissue engineering.

ACTIVITY REPORT
Research Activity

The research activity was mainly carried out at the IIT

Please indicate here if you have spent research periods in foreign countries.

Scientific Publications

Original publications on ISI Journals:

- 1) Caviglioli G., Baldassari S., Zuccari G., Yan Mengying., A.M. Bassi. *A three-dimensional hydrogel scaffold for cell culturing and a method for the production thereof*. Italian patent, titleholder: UNIGE, Application Number: 812017000109473;
- 2) Emma Piacentini., Mengying Yan., Lidietta Giorno. *Development of enzyme-loaded PVA microspheres by membrane emulsification*, Journal of Membrane Science 524 (2017) 79–86
- 3) Parodi B., Russo E., Baldassari S., Zuccari G., Pastorino S., Yan M., Neduri K., Caviglioli G. *Development and characterization of a mucoadhesive sublingual formulation for pain control: extemporaneous oxycodone films in personalized therapy*, Drug Development and Industrial Pharmacy, DOI: 10.1080/03639045.2017.1281290

Communications at Conferences

Oral communications:

- 1) "Characterization methods for cell culture hydrogel scaffolds", Advanced school in nanomedicine (25-28 September 2017, Pula, Cagliari)

Poster Communications:

- 1) "Injectable formulations for local administration of metformin hydrochloride", XXIII National Meeting in Medicinal Chemistry (6-9 September 2015, Campus University of Salerno, Fisciano)
- 2) "Study of Chitosan-Clodronate nanoparticles embedded in a thermoreversible gel based poloxamero", XV edition of Summer School in Pharmaceutical-Technological disciplines (9-11 September 2015, Campus of Fisciano, Department of Pharmacy)
- 3) "Development of gel formulations for localized release of metformin" 10th world meeting on pharmaceuticals, Biopharmaceutics and Pharmaceutical Technology (4-7 April 2016, Glasgow, United Kingdom)
- 4) "Norbiotinamine as coupling agent for pretargeting: improvement of preparative reaction (optimization)" XVI Summer school ,2° Corso permanente di aggiornamento per i dottorandi del settore Tecnologico-Farmaceutico "Farmaci Biotech: dall'idea alla pratica clinica" (5-8 September 2016, Uical, Department of pharmacy)
- 5) "Buccoadhesive polymeric films for oromucosal oxycodone delivery in acute pain control",XVI Summer school ,2° Corso permanente di aggiornamento per i dottorandi del settore Tecnologico-Farmaceutico "Farmaci Biotech: dall'idea alla pratica clinica" (5-8 September 2016, Uical, Department of pharmacy)
- 6) "Optimization of a parenteral thermoresponsive formulation based on metformin hydrochloride", 2nd European Conference on Pharmaceutics: Novel Dosage Forms, Innovative Technologies (3-4 April 2017, Krakow, Poland)
- 7) "Preformulation study of multilayer films for local treatment of oral diseases", Advanced school in nanomedicine (25-28 September 2017, Pula, Cagliari)

Congresses Attended

1. XXIII National Meeting in Medicinal Chemistry (6-9 September 2015, Campus University of Salerno, Fisciano)

2. 2nd European Conference on Pharmaceutics: Novel Dosage Forms, Innovative (3-4 April 2017, Krakow, Poland)

Courseware

During this 1st year ... has acquired ... credits of Courseware.

Courses attended and passed (11 credits)

Courses Given by Teachers of the Department of Pharmacy (University of Genoa)

- 1) Multivariate analysis of chemicals data (Teachers: Lanteri, Armanino, Leardi) (3 credits)
- 2) Molecular markers of food quality and genuineness (Teachers: Boggia, Zunin) (2 credits)
- 3) Ricerca bibliografica e brevettale nelle scienze farmaceutiche tramite banche dati (Teachers: P.Fossa, C.Brullo) (2 credits)
- 4) Metodi di preparazione e controllo di forme farmaceutiche innovative (Teachers: Caviglioli, Parodi, Russo, Baldassari, Zuccari) (2 credits)
- 5) Tecniche strumentali per la determinazione di elementi in traccia di interesse farmaceutico, alimentare, ambientale (Teachers: Minganti, Drava) (2 credits)

Courses given by invited experts:

- 1) "Solid State Modification: Principles and Applications for Drug Solubility Enhancement", Dr. Paolo Gatti (DIFAR 07/11/2014).
- 2) "New trends in computer aided drug design", Dr. Tiziano Tuccinardi (DIFAR 09/12/2014).
- 3) "X-ray based experimental techniques and characterization of nano-materials", Dr. Alberto Morgante (DCCI 31/03/2015)
- 4) "Medicinal chemistry with carbohydrates: the influenza virus and the discovery of sialidase inhibitors", Prof.ssa Anna Bernardi (DCCI 13/11/2015)

National and International Schools or Workshops

- 1) Colture Cellulari: I metodi alternativi (26-27 Febbraio 2015, DIMES-SEZIONE PATOLOGIA GENERALE, Genova)
- 2) Second Workshop on In-vitro Alternatives (23-24 Luglio 2015, IVTech srl e IFAC-CNR, Firenze)
- 3) XV Summer School in Pharmaceutical-Technological disciplines (9-11 September 2015, Campus di Fisciano, Department of Pharmacy).
- 4) Il Corso permanente di aggiornamento per I dottorandi del settore tecnologico-farmaceutico (5-8 September 2016, University of Calabria, Arcavacata di Rende, CS)
- 5) Dare un senso ai metodi sostitutivi alla sperimentazione animale (6-7 luglio 2017, DIMES Patologia Generale, Genova)
- 6) 3D printing and biofabrication (10-14 luglio 2017, University of Utrecht, Netherlands)
- 7) Advanced school in nanomedicine (25-28 September 2017, Pula, Cagliari)

Seminars Given

- 1)

Seminars Attended

- 1) "Biocatalysis: applications in pharmaceutical synthesis", Dr. Matteo Massa, (DIFAR 28/11/2014).

- 2) "Natural molecules and Xeno-hormesis", Dr. Giacomo Mele, (DIFAR 28/11/2014).
- 3) "Alternative methods to animal testing", Drs. Benedetta Pollarolo, (DIFAR 28/11/2014).
- 4) "Recent aspects of therapeutic interest in the process of tumor metastasis", Drs. Camilla Zibana, (DIFAR 28/11/2014).
- 5) "Tissue Engineering: dall'ingegneria alla biologia", Prof. Claudio Migliaresi, (DIMI, 10/04/2015)
- 6) "Neurons from stem cell: cognitive and clinical prospects in neurology", Sen. Elena Cattaneo, (Auditorium CBA 24/04/15).
- 7) "Terapia cellulare per le distrofie muscolari: risultati clinici e la via verso l'efficacia" Prof. Giulio Cossu, (Auditorium CBA 06/05/2015)
- 8) "Models for the in vitro study of human metabolism", Prof. Arti Ahluwalia, (Polo Alberti 16/07/15).
- 9) "Il sistema biotina-(strept) avidina nel pretargeting e in applicazioni biotecnologiche, The Biotin-(Strept) avidin system in pretargeting and in biotechnological applications," Dott.ssa Irene Croce, (DIFAR 27/11/2015)
- 10) "Tecnologie avanzate per lo sviluppo di modelli alternative fisiologicamente rilevanti in vitro, Advanced technologies for the development of physiologically relevant in vitro alternative models," Dott.ssa Jenia Danailova, (DIFAR 27/11/2015)
- 11) "Reazioni palladio-catalizzate: un impatto rivoluzionario in chimica farmaceutica, Palladium-catalyzed reactions: a revolutionary impact in medicinal chemistry," Dott. Andrea Desogus, (DIFAR 27/11/2015)
- 12) "Rivoluzione nella terapia delle malattie parassitarie:artemisinina come grande successo scientifica, Revolution in the treatment of parasitic diseases: Artemisinin as great scientific goal.Dott.ssa Cinzia M. Francini,(DIFAR 27/11/2015)
- 13) "Druglikeness e metodi di score relativi: Ligand efficiency e lipophilic ligand efficiency. Druglikeness and related scoring methods: ligand efficiency and lipophilic ligand efficiency." Dott.ssa Sara Guariento,(DIFAR 27/11/2015)
- 14) "L'analisi termica per la caratterizzazione dei polimeri, dei compositi e delle resine con dimostrazioni pratiche DSC e DEA." Netzsch,(Milan 12/04/2016)
- 15) "Odori, profumi e feromoni come mediatori chimici olfattivi", Chiara Lacapra, (DIFAR 18/11/2016)
- 16) "Tubercolosi ed altre patologie polmonari: stato dell'arte e recenti sviluppi terapeutici", Elda Meta, (DIFAR 18/11/2016)
- 17) "Giocare sporco: PAINS e composti promiscui", Anita Parricchi, (DIFAR 18/11/2016)
- 18) "Il marketing cosmetico: dalla mission aziendale alla risposta del consumatore", Silvia Rum, (DIFAR 18/11/2016)
- 19) "Cancer Tissue Engineering: new technological approaches for providing alternative 3-dimensional in vitro tumor models for cancer biology and drug testing", Prof.ssa Silvia Scaglione,(DIMES 19/04/2017)

Other Activities

- 1) Laboratory assistance in Technology, Socioeconomy and Pharmaceutical Legislation II (CTF), 30 hours, a.a. 2015/2016 (first semester).
- 2) Laboratory assistance in Technology, Socioeconomy and Pharmaceutical legislation I (Far), 30 hours, a.a. 2016/2017 (first semester).

Yan Meng ying

20.10.2017