

UNIVERSITY OF GENOVA

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

XXVI CYCLE YEARBOOK

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

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

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

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

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

Research structure and teaching staff

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

Internationalization

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

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

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

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

Adriana Saccone
Director of the Course

MANAGEMENT COUNCILS OF THE COURSE

The course was governed by a Board of Professors, formed by 32 members, and by a Director.

For the XXXI 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 Pharmacy (DIFAR), Department of Civil, Chemical and Environmental Engineering (DICCA), Department of Physics (DIFI), Italian Institute of Technology (IIT)

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

COURSEWARE

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

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

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



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



Curriculum: Nanochemistry

QUINTEN A. AKKERMAN

Start of the Doctorate Program: November 1st, 2015

End of the Doctorate Program: October 31st, 2018

Advisors: Prof. Liberato Manna (IIT), Prof. Gabriele Cacciamani (ige) &
Dr. Mirko Prato (IIT)

Thesis Title: Perovskite Nanocrystals: From size, shape and composition control to optoelectronic applications

Thesis abstract

Lead halide based perovskite semiconductors have recently gained wide interest following their successful embodiment in solid state photovoltaic devices with impressive power conversion efficiencies (now above 20%), while offering a relatively simple and low cost processability. While, on one hand, the primary optoelectronic properties of these materials have already met the requirement for high efficiency optoelectronic technologies, the poor control of their growth processes in thin films represents, to date, a major roadblock for market exploitation. While the majority of research has focused on thin films, colloidal hybrid organic-inorganic or to fully inorganic perovskite nanocrystals (NCs) have only been developed very recently. This thesis focuses on the size, shape and composition control of lead halide perovskite and metal halide nanocrystals, as well as their application in optoelectronic devices.

ACTIVITY REPORT

Research Activity

Research Period Abroad

Molecular Foundry, Berkeley, USA (July-September 2017)

Scientific Publications

First author:

1. **Akkerman, Q. A.**; Motti, S. G.; Srimath Kandada, A. R.; Mosconi, E.; D'Innocenzo, V.; Bertoni, G.; Marras, S.; Kamino, B. A.; Miranda, L.; De Angelis, F.; Petrozza, A.; Prato, M.; Manna, L., Solution Synthesis Approach to Colloidal Cesium Lead Halide Perovskite Nanoplatelets with Monolayer-Level Thickness Control. *J. Am. Chem. Soc.* **2016**, *138*, 1010-1016.

2. **Akkerman, Q. A.**; Gandini, M.; Di Stasio, F.; Rastogi, P.; Palazon, F.; Bertoni, G.; Ball, J. M.; Prato, M.; Petrozza, A.; Manna, L., Strongly Emissive Perovskite Nanocrystal Inks for High-Voltage Solar Cells. *Nat. Energy* **2016**, *2*, 16194.
3. **Akkerman, Q. A.**; Park, S.; Radicchi, E.; Nunzi, F.; Mosconi, E.; De Angelis, F.; Brescia, R.; Rastogi, P.; Prato, M.; Manna, L., Nearly Monodisperse Insulator Cs₄PbX₆ (X = Cl, Br, I) Nanocrystals, Their Mixed Halide Compositions, and Their Transformation into CsPbX₃ Nanocrystals. *Nano Lett.* **2017**, *17*, 1924-1930.
4. **Akkerman, Q. A.**; Meggiolaro, D.; Dang, Z.; De Angelis, F.; Manna, L., Fluorescent Alloy CsPb_xMn_{1-x}I₃ Perovskite Nanocrystals with High Structural and Optical Stability. *ACS Energy Lett.* **2017**, *2*, 2183-2186.
5. **Akkerman, Q. A.**; Rainò, G.; Kovalenko, M. V.; Manna, L., Genesis, Challenges and Opportunities for Colloidal Lead Halide Perovskite Nanocrystals. *Nat. Mater.* **2018**, *17*, 394-405.
6. **Akkerman, Q. A.**; Abdelhady, A. L.; Manna, L., Zero-Dimensional Cesium Lead Halides: History, Properties, and Challenges. *J. Phys. Chem. Lett.* **2018**, *9*, 2326-2337.
7. **Akkerman, Q. A.**; Martínez-Sarti, L.; Goldoni, L.; Imran, M.; Baranov, D.; Bolink, H. J.; Palazon, F.; Manna, L., Molecular Iodine for a General Synthesis of Binary and Ternary Inorganic and Hybrid Organic-Inorganic Iodide Nanocrystals. *Chem. Mater.* **2018**, *30*, 6915-6921.

Other publications:

1. Palazon, F.; **Akkerman, Q. A.**; Prato, M.; Manna, L., X-Ray Lithography on Perovskite Nanocrystals Films: From Patterning with Anion-Exchange Reactions to Enhanced Stability in Air and Water. *ACS Nano* **2016**, *10*, 1224-1230.
2. Palazon, F.; Di Stasio, F.; **Akkerman, Q. A.**; Krahne, R.; Prato, M.; Manna, L., Polymer-Free Films of Inorganic Halide Perovskite Nanocrystals as Uv-to-White Color-Conversion Layers in Leds. *Chem. Mater.* **2016**, *28*, 2902-2906.
3. Srimath Kandada, A. R.; Neutzner, S.; D'Innocenzo, V.; Tassone, F.; Gandini, M.; **Akkerman, Q. A.**; Prato, M.; Manna, L.; Petrozza, A.; Lanzani, G., Nonlinear Carrier Interactions in Lead Halide Perovskites and the Role of Defects. *J. Am. Chem. Soc.* **2016**, *138*, 13604-13611.
4. Dang, Z.; Shamsi, J.; Palazon, F.; Imran, M.; **Akkerman, Q. A.**; 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*, 2124-2132.
5. Palazon, F.; Almeida, G.; **Akkerman, Q. A.**; De Trizio, L.; Dang, Z.; Prato, M.; Manna, L., Changing the Dimensionality of Cesium Lead Bromide Nanocrystals by Reversible Postsynthesis Transformations with Amines. *Chem. Mater.* **2017**, *29*, 4167-4171.
6. Lorenzon, M.; Sortino, L.; **Akkerman, Q.**; Accornero, S.; Pedrini, J.; Prato, M.; Pinchetti, V.; Meinardi, F.; Manna, L.; Brovelli, S., Role of Nonradiative Defects and Environmental Oxygen on Exciton Recombination Processes in CsPbBr₃ Perovskite Nanocrystals. *Nano Lett.* **2017**, *17*, 3844-3853
7. Di Stasio, F.; Imran, M.; **Akkerman, Q. A.**; 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*, 2725-2729.
8. Meinardi, F.; **Akkerman, Q. A.**; Bruni, F.; Park, S.; Mauri, M.; Dang, Z.; Manna, L.; Brovelli, S., Doped Halide Perovskite Nanocrystals for Reabsorption-Free Luminescent Solar Concentrators. *ACS Energy Lett.* **2017**, 2368-2377.
9. Palazon, F.; Urso, C.; De Trizio, L.; **Akkerman, Q.**; Marras, S.; Locardi, F.; Nelli, I.; Ferretti, M.; Prato, M.; Manna, L., Postsynthesis Transformation of Insulating Cs₄PbBr₆ Nanocrystals into Bright

- Perovskite CsPbBr₃ through Physical and Chemical Extraction of CsBr. *ACS Energy Lett.* **2017**, 2445-2448.
10. Dang, Z.; Shamsi, J.; **Akkerman, Q. A.**; Imran, M.; Bertoni, G.; Brescia, R.; Manna, L., Low-Temperature Electron Beam-Induced Transformations of Cesium Lead Halide Perovskite Nanocrystals. *ACS Omega* **2017**, 2, 5660-5665.
 11. Almeida, G.; Goldoni, L.; **Akkerman, Q.**; Dang, Z.; Khan, A. H.; Marras, S.; Moreels, I.; Manna, L., Role of Acid-Base Equilibria in the Size, Shape, and Phase Control of Cesium Lead Bromide Nanocrystals. *ACS Nano* **2018**, 12, 1704-1711.
 12. Palazon, F.; Chen, F.; **Akkerman, Q. A.**; Imran, M.; Krahn, R.; Manna, L., Effects of Oxygen Plasma on the Chemical, Light-Emitting, and Electrical-Transport Properties of Inorganic and Hybrid Lead Bromide Perovskite Nanocrystal Films. *ACS Applied Nano Materials* **2018**.

Communications at Conferences

Oral communications:

1. PSCO 2016, Lausanne (Switzerland), 2015
2. ISN2A, Lisbon (Portugal), 2016
3. MRS, Phoenix (Unites States), 2016
4. AP-HOPV17, Yokohama (Japan), 2017
5. (Invited) Colloidal Semiconductor Nanocrystals (GRS), Smithfield (United States), 2018
6. (Invited) E-MRS Fall Meeting, Warsaw (Poland), 2018

Poster Communications:

1. ISN2A, Lisbon (Portugal), 2016
2. Nanax7, Marburg (Germany), 2016
3. FQDots16, Berlin (Germany), 2016
4. PSCO 2016, Genova (Italy), 2016
5. AP-HOPV17, Yokohama (Japan), 2017
6. Molecular Foundry use meeting, Berkeley (USA), 2017

Congresses Attended

1. PSCO 2016, Lausanne (Switzerland), 2015
2. ISN2A, Lisbon (Portugal), 2016
3. Nanax7, Marburg (Germany), 2016
4. FQDots16, Berlin (Germany), 2016
5. PSCO 2016, Genova (Italy), 2016
6. MRS, Phoenix (Unites States), 2016
7. AP-HOPV17, Yokohama (Japan), 2017
8. Molecular Foundry use meeting, Berkeley (USA), 2017
9. Colloidal Semiconductor Nanocrystals (GRS), Smithfield (United States), 2018
10. E-MRS Fall Meeting, Warsaw (Poland), 2018

Courseware

Courses attended and passed

1. Struttura elettronica dei solidi
Taught by: Libero Manna
Credits: 1

2. Basics of Crystallography and Diffraction by crystals
Taught by: Mirko Prato
Credits: 1
3. Opto-Electronic Properties of Semiconductor Quantum Dots
Taught by: Iwan Moreels
Credits: 1
4. Magnetic properties and characterization techniques
Taught by: Aidin Lak
Credits: 1
5. Tecniche di caratterizzazione (XPS), Raman, FTIR, NMR
Taught by:
Credits: 1
6. The application of Nanocrystals in energy storage, photo-catalysis and heterogeneous catalysis
Taught by: Massimo Colombo, Dipak Shinde, Simone Monaco
Credits: 1
7. Science and technology of 2D crystals
Taught by: Francesco Bonaccorso
Credits: 1
8. Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations
Taught by: Luca De Trizio
Credits: 1
9. Introductory course on transmission electron microscopy
Taught by: Rosaria Brescia, Zhiya Dang, Joka Buha, Roberto Marotta
Credits: 1

Courses Given by invited experts:

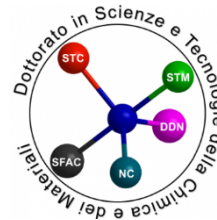
1. Nanoparticles Chemistry for the use of energy conversion and theranostics
Taught by: Clemens Burda
Credits: 1 credit

National and International Schools or Workshops

1. International Summer School on Photovoltaics and New Concepts of Quantum Solar Energy Conversion (Quantsol), September 2-9, Hirschegg, Austria, 2018



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



Curriculum: Chemical Sciences and Technologies

MANUEL ANSELMO

Start of the Doctorate Program: November 1st, 2015

End of the Doctorate Program: October 31st, 2018

Advisors: Prof. Andrea Basso (Unige), Prof. Burkhard Konig (internship)

Thesis Title: Exploitation of Photchemistry and Photoredox Catalysis towards novel transformations in Organic Synthesis: multicomponent reactions, synthesis of heterocycles and other applications.

Thesis abstract

A novel approach towards the synthesis of complex 5-,6- and 7- membered lactones via photoredox catalysis exploiting arenediazonium tetrafluoroborates is reported. Consequential serendipitous discovery of the generation of the acetyl radical in photoredox catalyzed conditions is described together with relative synthetic applications. Intertwined research on the photoinduced multicomponent synthesis of α -silyloxy acrylamides as an unexplored class of silyl enol ethers is also reported.

ACTIVITY REPORT

Research Activity

Research Period Abroad

4 October 2017 - 23 March 2018, Università di Regensburg, Germania, Gruppo di Ricerca del Prof. Burkhard Koenig

Scientific Publications

1. 'Photocatalyzed synthesis of isochromanones and isobenzofuranones under batch and flow conditions'. Anselmo, M.; Moni, L.; Ismail, H.; Comoretto, D.; Riva, R.; Basso, A., *Beilstein J. Org. Chem.* **2017**, *13*, 1456-1462.

2. 'Photoinduced Multicomponent Synthesis of α - Silyloxy Acrylamides, an Unexplored Class, of Silyl Enol Ethers'. Ibba, F.; Capurro, P.; Garbarino, S.; **Anselmo, M.**; Moni, L.; Basso, A. *Org. Lett.* **2018**, *20*, 4, 1098-1101.
3. Contribution to the book: 'Photoorganocatalysis in Organic Synthesis', authors Fagnoni, M.; Protti, S.; Ravelli, D., <https://doi.org/10.1142/q0180>, ISBN: 978-1-78634-604-9
4. Contribution, coauthor of the Chapter: 'Photoorganocatalysis in Flow', Moni, L.; **Anselmo, M.**; Basso, A., publishing planned for January 2019.
5. 'Photoredox catalyzed generation of acetyl radical in flow: theoretical investigation, and synthetic applications'. Anselmo, M.; Basso, A.; Protti, S.; Ravelli, D., submitted paper

Communications at Conferences

Oral communications:

1. 'Highly Convergent Synthesis of Intensively Blue Emissive Furo[2,3-c]isoquinolines by a Palladium-Catalyzed Cyclization Cascade of Unsaturated Ugi Products' 5-8/06/2016, Genova: 'XII Congresso del gruppo interdivisionale di Chimica Organometallica, Genova, COGICO 2016'
2. 'Photocatalyzed synthesis of isochromanones and isobenzofuranones under batch and flow conditions' 18-22/06/2017 Gargnano: 'International School on Organic Synthesis 'A. Corbella' ISOS 2017'
3. 'Photoredox Dual-Catalyzed generation and trapping of aliphatic acyl radicals' 10-14/06/2018 Gargnano: 'International School on Organic Synthesis 'A. Corbella' ISOS 2018'

Poster Communications:

1. 'Photocatalyzed synthesis of isochromanones and isobenzofuranones under batch and flow conditions' 2-6/07/2017, Koln: '20th European Symposium on Organic Chemistry ESOC 2017'

Congresses Attended

1. 5-8/06/2016, Genova: 'XII Congresso del gruppo interdivisionale di Chimica Organometallica, Genova, COGICO 2016'
2. 2-6/07/2017, Koln: '20th European Symposium on Organic Chemistry ESOC 2017'

Courseware

Type A courses:

1. 13/11/2015 DCCI, Genova: 'Medicinal chemistry with carbohydrates: the influenza virus and the discovery of sialidase inhibitors' Prof. Anna Bernardi (Università di Milano) !
2. 27/11/2015 DCCI, Genova: ' New Methods for food authenticity and safety testing' Dr. Valeria Merlo (Direzione tecnica Eurofins, Cuneo) !
3. 9-10/06/2016 DCCI, Genova: 'Functional chromophores - syntheses and applications' Prof. Thomas J. J. Muller (Heinrich-Heine University, Dusseldorf)

Type B courses:

1. Analisi Multivariata dei dati Chimici
Prof. Monica Casale, Prof. Riccardo Leardi, Prof. Paolo Olivieri
Credits: 3
2. Fotochimica Organica
Prof. Andrea Basso
Credits: 2

3. Chimica Bioorganica
Prof. Luca Banfi
Credits: 2
4. Materiali Organici per la l'Elettronica, la Fotonica e l'Optoelettronica
Prof. Davide Comoretto
Credits: 2
5. Metodologie della Ricerca Sperimentale
Prof. Marco Grotti, Prof. Riccardo Leardi
Credits: 3
6. Chimica Bioinorganica
Prof. Serena De Negri
Credits: 2
7. Sintesi Orientata alla Diversità di Composti Eterociclici
Prof. Renata Riva, Dr. Lisa Moni
Credits: 2

Seminars

1. 7/06/2018 DCCI, Genova 'Ligands for functional targeting of G-Quadruplex nucleic acids' Prof. Mauro Freccero
2. 6/11/2015 DCCI, Genova 'Artificial Metalloenzymes: combining metal- and biocatalysis for organic synthesis' Erika Tassano (Dottoranda DCCI XXVIII ciclo)
3. 9/06/2016 DCCI, Genova 'Diversity oriented synthesis of functional dyes- novel sequences, novel structures, novel properties' Prof. Thomas J. J. Muller (Heinrich-Heine University, Dusseldorf)
4. 30/09/2016 IIT, Genova: 'Fragment-based drug discovery for identifying single- and multi-target inhibitors of CNS targets' Prof. Anders Bach (University of Copenhagen)
5. 12/06/2017 DCCI, Genova: 'Un caso di proficua collaborazione: biocatalisi e prodotti naturali' Dr. Sergio Riva (Direttore Istituto di Chimica del Riconoscimento Molecolare del CNR, Milano)
6. 04/06/2018 DCCI, Genova: "Targeting the purinergic signaling in the heart. New perspectives for understanding the electrophysiological role of adenosine in atrial fibrillation" Dr. Luca Soattin (PhD candidate Cardiac Physiology Laboratory – Københavns Universitet) !
7. Ciclo di seminari conclusivi dell'attività di dottorato e difesa della tesi di dottorato di Erika Tassano, Martina Spallarossa, Silvia Garbarino e Samantha Caputo
8. Ciclo di seminari svolti presso la sezione di Chimica Organica dell'Università di Regensburg a frequenza settimanale nel periodo 4 October 2017 - 23 March 2018 (24 settimane).

National and International Schools or Workshops !

1. 17/02/2016 DCCI, Genova: 'International Workshop on Industrial Waste (IWIW 2016)'
2. 18-22/06/2017 Gargnano: 'International School on Organic Synthesis 'A. Corbella' ISOS 2017'
3. 10-14/06/2018 Gargnano: 'International School on Organic Synthesis 'A. Corbella' ISOS 2018'

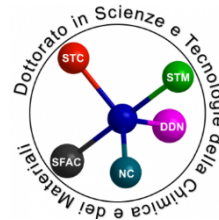
Teaching support

- Inizio – fine attività: 06.04.2016 – 15.10.2016 n. 30 ore di supporto a insegnamento di Chimica Organica 2, modulo 1 Cod. 65109 (L CTC)
- Inizio – fine attività: 16.10.2016 – 31.12.2016 n. 30 ore di supporto a insegnamento di Chimica Organica 2, modulo 1 Cod. 65111 (L CTC)

- Ho seguito Miss Deianira Lanteri durante il suo lavoro di tirocinio triennale (Giugno-Luglio 2016) e nella stesura della sua relazione di tirocinio.
- Ho seguito Mr Hossny Ismail Yosri (Febbraio-Luglio 2017) durante il suo lavoro di tesi di Laurea Magistrale e nella stesura della sua tesi. Ho inoltre seguito Mr. Yosri durante un suo periodo di lavoro come volontario (Settembre 2017) nel Gruppo di ricerca di chimica BioOrganica (BOG) del DCCI sotto la supervisione del Prof. Andrea Basso.
- Ho seguito Mr Gabriele Descisciolo durante il suo lavoro di tirocinio triennale (Luglio-Settembre 2018) e nella stesura della sua relazione di tirocinio.
- Ho seguito Miss Alessa Rolka durante il suo lavoro di tirocinio triennale (Novembre-Dicembre 2017) nella struttura straniera dell'Università di Regensburg.



Università degli Studi di Genova
Doctorate in
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Curriculum: Scienze e tecnologie Chimiche

BARBARA BENEDETTI

Start of the Doctorate Program. November 1st, 2015

End of the Doctorate Program: October 31st, 2018

Advisor: Prof. Emanuele Magi

Thesis Title: Development and optimization of innovative analytical methods for the determination of phytoestrogens in soy-food by chromatographic techniques coupled to mass spectrometry

Thesis abstract

My thesis is based on the development and validation of innovative analytical methodologies for the extraction and quantitative analysis of endocrine disrupting chemicals (EDCs), substances that have been discovered to be concerning for human health in the latest years. In particular, the work focused on a class of natural substances, phytoestrogens, which are found in the plant kingdom and are considered EDCs. Different extraction methods combined with GC-MS and LC-MS were studied and optimized for the determination of phytoestrogens in soy-foods. Alongside this topic, an innovative method for the determination of more “classical” contaminants, namely polycyclic aromatic hydrocarbons, was developed.

ACTIVITY REPORT
Research Activity

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

Research Period Abroad

Research stay in Barcellona (Spain), laboratory of professor Silvia Diaz Cruz, IDAEA, CSIC. Start: 1st September 2017; End: 1st November 2017

Scientific Publications

Original publications on ISI Journals:

1. Emanuele Magi, Marina Di Carro, Cristiana Mirasole, **Barbara Benedetti**. Combining passive sampling and tandem mass spectrometry for the determination of pharmaceuticals and other emerging pollutants in drinking water. *Microchemical Journal*, 136C (2018) pp. 56-60. <https://doi.org/10.1016/j.microc.2016.10.029>.
2. **Barbara Benedetti**, Marina Di Carro, Cristiana Mirasole, Emanuele Magi. Fast derivatization procedure for the analysis of phytoestrogens in soy milk by gas chromatography tandem mass spectrometry. *Microchemical Journal*, 137 (2018) pp. 62–70. <https://doi:10.1016/j.microc.2017.09.023>.
3. **Barbara Benedetti**, Marina Di Carro, Emanuele Magi. Phytoestrogens in soy-based meat substitutes: Comparison of different extraction methods for the subsequent analysis by liquid chromatography-tandem mass spectrometry, *Journal of Mass Spectrometry* 53 (2018) pp. 862-870. <https://doi:10.1002/jms.4268>.

Communications at Conferences

Oral communications:

1. Marina Di Carro, Cristiana Mirasole, **Barbara Benedetti** and Emanuele Magi. Pharmaceuticals and other emerging pollutants: combining passive sampling and tandem mass spectrometry for their determination in water. "Book of abstracts", pag. 93, ISBN 978-88-6741-659-2, XV Italian-Ungarian Symposium on Spectrochemistry-pharmacological research and analytical approaches, June 12-16 2016, Pisa, Italy.
2. **Barbara Benedetti**, Marina Di Carro, Cristiana Mirasole and Emanuele Magi. Analysis of phytoestrogens by GC-MS/MS: method development and application to soy drinks. "Proceedings", pag 62, 2nd NatMedDay, June 28-30 2017, Sansepolcro (AR), Italy.
3. **Barbara Benedetti**, Marina Di Carro, Emanuele Magi. Extraction of phytoestrogens from soy milk and soy-based meat substitutes and quantitation by liquid chromatography coupled to tandem mass spectrometry. Proceedings of the 5th MS Food Day, OR23, pag. 94-96, ISBN: 9788890738838, October 11-13, 2017, Bologna.
4. **Barbara Benedetti**, Marina Di Carro, Emanuele Magi. Multivariate optimization of a QuEChERS procedure for the LC-MS/MS analysis of phytoestrogens in soy burgers. Abstract book of the XXVII Congress of the Analytical Division (SCI), Flash oral communication F2 FN, ISBN 978-88-94952-04-9, September 16-20, 2018, Bologna.

Poster Communications:

1. **Benedetti Barbara**, Di Carro Marina, Mirasole Cristiana, Magi Emanuele. Analysis of phytoestrogens by GC-MS/MS: study of the instrumental conditions and derivatization procedure. "Abstract book" P18 pag. 64, ISSN: 0393-5620, Massa 2016, September 6-8, 2016, Roma, Italy.
2. Magi Emanuele, Di Carro Marina, Mirasole Cristiana, **Benedetti Barbara**. Determination of emerging pollutants in water: The passive sampling approach, Proceedings XXVI Congresso Nazionale di Chimica Analitica (SCI), P28 pag. 195 ISBN: 978-88-86208-91-8, September 18-22 2016, Giardini Naxos (ME).
3. Magi Emanuele, Di Carro Marina, Benedetti Barbara. A simple and rapid GC-MS/MS method for the determination of phytoestrogens in soy drinks, XXVI Congresso Nazionale della SCI, Paestum (SA) September 10 -14, 2017

4. Marina Di Carro, **Barbara Benedetti**, Emanuele Magi. Study of the volatile fraction of edible pine nuts by HS-SPME-GC-MS. Proceedings of the 5th MS Food Day, P66, pag. 319-320, ISBN:9788890738838, October 11-13, 2017, Bologna.
5. **Benedetti Barbara**, Di Carro Marina, Magi Emanuele. Polycyclic aromatic hydrocarbons in sea water: extraction by magnetic molecular imprinted microparticles for their determination by GC-MS. Abstract book of the 42nd International Symposium on Capillary Chromatography, poster C17, pag. 206, ISBN: 978-88-941816-1-6, May 15-18, 2018, Riva del Garda (TN).
6. **Benedetti Barbara**, Di Carro Marina, Magi Emanuele. Multivariate study of matrix effect in the analysis of phytoestrogens in soy-food by LC-ESI-MS/MS. XXII International Mass Spectrometry Conference 2018, August 26-31, 2018, Firenze.

Congresses Attended

1. XV Italian-Ungarian Symposium on Spectrochemistry-pharmacological research and analytical approaches, June 12-16, 2016, Pisa, Italy.
2. Massa 2016, September 6-8, 2016, Roma, Italy.
3. 3th MS-EnviDay, September 26-28, 2016, Livorno, Italy.
4. 5th MS J-Day "I giovani e la spettrometria di massa", November 24 2016, Pisa, Italy
5. 2nd NatMedDay, June 28-30, 2017, Sansepolcro (AR), Italy.
6. 5th MS Food Day, October 11-13, 2017, Bologna, Italy.
7. 42nd International Symposium on Capillary Chromatography, May 15-18, 2018, Riva del Garda (TN), Italy.
8. XXII International Mass Spectrometry Conference 2018, August 26-31, 2018, Firenze, Italy.
9. XXVII Congress of the Analytical Division (SCI), September 16-20, 2018, Bologna, Italy.

Courseware

Courses attended and passed

1. Metodologia della ricerca sperimentale.
Prof. Leardi, Prof. Grotti
3 credits
2. Principali piante utilizzate in Fitocosmesi e loro costituenti.
Prof. Bisio
2 credits
3. Tecniche strumentali per la determinazione di elementi in traccia di interesse farmaceutico, alimentare, ambientale.
Prof. Minganti
2 credits
4. Analisi multivariata dei dati chimici.
Prof. Leardi, Casale, Oliveri
3 credits
5. Marker molecolari della qualità e della genuinità degli alimenti.

Prof. Boggia, Prof.Zunin

2 credits

Courses Given by invited experts:

1. "Functional chromophores – syntheses and applications". June 9-10, 2016, Prof. Thomas J.J. Müller (type A course- 1 credit)
2. "Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials" and "Novel Materials for energy storage and conversion" May 11, 2017, Prof. Thomas Fässler (type A course- 1 credit)
3. "Approaches to synthesis and characterization of magnetic nanomaterials for biomedical applications" Jan 23-24 2018, Dr. Davide Peddis (type A course- 1 credit)

Seminars Attended

1. "Multi-block regression and classification based on PLS regression and extensions" May 23 2016, prof. Tormod Naes
2. "New trends in Computer aided drug design" October 18 2016, Dr. Tiziano Tuccinardi
3. "Il marketing cosmetico: dalla mission aziendale alla risposta del consumatore", November 18 2016, Dr.ssa Silvia Rum
4. "Odori, profumi e feromoni come mediatori chimici olfattivi", November 18 2016, Dr.ssa Chiara Lacapra
5. "Giocare sporco: PAINS e composti promiscui", November 18 2016, Dr.ssa Anita Parricchi
6. "Tubercolosi ed altre patologie polmonari: stato dell'arte e recenti sviluppi terapeutici", November 18 2016, Dr.ssa Elda Meta
7. "Exploring the transformation mechanisms of matter at the nanoscale with computer simulations", November 21 2016, Fabio Pietrucci
8. "Dal problema astronomico alla strumentazione: essere a meta' tra scienza e tecnologia", February 03 2017, Dr Marco Landoni
9. "Fotopolimeri in astronomia: aspetti pratici e risultati in cielo", February 03 2017, Dr Alessio Zanutta
10. "Sviluppo di nuovi materiali per olografia: dalla molecola al materiale", February 03 2017, Dr Andrea Bianco
11. "Atomic structure and mass-production of size-selected nanoparticles (clusters)", May 30 2017, prof. Richard E. Palmer
12. "Analisi termica accoppiata alla gas cromatografia e spettrometria di massa. Un potente strumento per la caratterizzazione dei materiali", June 13, 2017, Dr Federico Locardi
13. "Design of magnetic nano-architecture for biomedical applications". January 24, 2018, Dr. Davide Peddis
14. "Il contributo del DCCI al Programma Nazionale di Ricerche in Antartide". February 27, 2018, Prof. Marco Grotti, Paola Rivaro
15. "Elettroni, fotoni e altre particelle: un viaggio nel mondo delle Particelle Fondamentali e delle Onde Gravitazionali" May 03, 2018, Prof. Luciano Maiani
16. "Food by-product as promise cosmetic active ingredient: a case study", May 04, 2018, Dr. Francisca Rodrigues

National and International Schools or Workshops

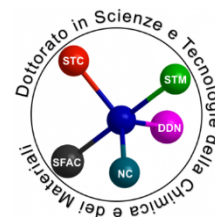
1. 20° Corso di Spettrometria di Massa, March 12-18 2016, Certosa di Pontignano (Siena), Italy

2. International workshop on industrial waste, February 17 2016, DCCI, Università di Genova, Genova
3. Scuola di experimental design, 4-8 giugno 2018, Genova

Other Activities

1. Supporto alla didattica: 40 ore di supporto per l'insegnamento "Chimica analitica I" a.a. 2015-2016, 06/04/2016-26/05/2016
2. Supporto alla didattica: 40 ore di supporto per l'insegnamento "Chimica analitica I" a.a. 2016-2017, 08/03/2017-31/05/2017

Attività di tutorato (tutor didattico): 30 ore per l'insegnamento "Chimica generale e inorganica" per il corso di laurea in Geologia (progetto A _SMFN_06) 06/11/2017-31/01/201



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

Curriculum: Nanochemistry

ALBERTO CAMISASCA

Start of the Doctorate Program: *November 1st, 2015*

End of the Doctorate Program: *October 31st, 2018*

Advisors: Prof. Silvia Giordani (IIT), Prof. Fabio Canepa (UniGe)

Thesis Title: "Synthesis of functionalized carbon nano-onions for high-resolution biological imaging and electrocatalysis"

Thesis abstract:

Carbon nanomaterials (CNMs) are a class of low-dimensional materials that have aroused a great deal of interest in the past 30 years since the spectacular debut of fullerene, the first member of this class reported by Smalley, Kroto, Curl et al. in 1985. The past decade has witnessed a burst in several research fields using CNMs, which are advantageous primarily owing to small size, unique optical properties, and large surface area; promising results in applications such as biomedical and electrochemical have shown the potentiality of these nanostructured materials.

The development of novel fluorescent systems for bio-imaging applications is a research field of increasing interest. Fluorescent-based biomedical imaging has the advantages of fast feedback, high sensitivity and resolution, but is limited by tissue penetration. Many efforts have been involving both investigation and further implementation of imaging agents for the biologically relevant near-infrared (NIR) region, where tissues exhibit minimal absorbance. This strategy allows for a deeper light absorption, proposing an innovative approach compared to the traditional visible imaging techniques. Carbon based nanomaterials emerged over the last few years as important imaging agents for biomedical applications because the size, typically ranging from 1 nm to 1 μm in size, is comparable to the that of relevant biological entities such as proteins (1–100 nm) and DNA (2–3 nm in width), making them ideal for biological applications.

CNMs have been also proposed as efficient cathode materials for electrocatalytic processes, due to large specific surface area (thus providing additional catalytic sites), cost effectiveness and outstanding electrical and mechanical properties. Nowadays, the development of new, clean and renewable energy technologies with high efficiency and cost-effectiveness is of utmost importance due to the increasing energy demand in our society. Fuel cells is one of the most promising strategies proposed to solve the energy-related problems, but its performance are limited by the kinetically slow oxygen reduction reaction at the cathode side. In addition, the standard catalyst (i.e. carbon-supported platinum) suffers from several drawbacks, thus precluding a possible commercialization. Therefore, many efforts were made to develop novel ORR catalysts.

One efficient strategy to increase the catalytic properties of CNMs is to introduce heteroatoms such as nitrogen into the graphitic lattice. The doping with non-metal heteroatoms (i.e. nitrogen, boron, sulphur and phosphorus) can efficiently improve the performance of the CNM-based catalysts due to the formation of active sites in the graphitic skeleton together with the synergistic coupling effects between heteroatoms.

Among the several members of the carbon family, carbon nano-onions (CNOs) showed very attractive features in different research fields, in particular in biomedical and electrochemical applications. CNOs are nearly spherical carbon nanoparticles composed of multiple nested fullerene-like shells with size and physico-chemical properties related to the method used for the fabrication.

My PhD project is focused on the synthesis of functionalized carbon nano-onions for the development of novel biological imaging systems and highly performing electrocatalysts.

ACTIVITY REPORT

Research Activity

The research activity was carried out at the IIT Genova from November 1st 2015 to March 31st 2017. From April 1st 2017 to October 31th 2018, the research activity was carried out at the IIT Torino.

Research activity abroad

From November 3rd 2016 to January 30th 2017, the research activity was carried out at the Bio-Nano Electronics Research Centre at Toyo University in Tokyo, Japan.

From April 30th to October 31st 2018, the research activity was carried out at Dublin City University (DCU) in Dublin, Ireland.

Scientific publications

Original publications on ISI Journals:

1. "Boron/Nitrogen-Codoped Carbon Nano-Onion Electrocatalysts for the Oxygen Reduction Reaction", **A. Camisasca**, A. Sacco, R. Brescia and S. Giordani, ACS Appl. Nano Mater.; DOI: 10.1021/acsanm.8b01430.
2. "Carbon nano-onions in biomedical applications: Promising theranostic agents", **A. Camisasca** and S. Giordani, Inorg. Chim. Acta 2017, 468, 67-76; doi: <https://doi.org/10.1016/j.ica.2017.06.009>.
3. "Far-Red Fluorescent Carbon Nano-Onions As Biocompatible Platform For Cellular Imaging", S. Lettieri, **A. Camisasca**, M. d'Amora, A. Diaspro, T. Uchida, Y. Nakajima, K. Yanagisawa, T. Maekawa and S. Giordani, RSC Adv. 2017, 7, 45676-45681; doi:10.1039/C7RA09442F.
4. "Toxicity Assessment of Carbon Nanomaterials in Zebrafish during Development", M. d'Amora, **A. Camisasca**, S. Lettieri and S. Giordani, Nanomaterials 2017, 7(12), 414; doi:10.3390/nano7120414.
5. "Carbon Nano-onions as Fluorescent On/Off Modulated Nanoprobes for Diagnostics", S. Lettieri, M. d'Amora, **A. Camisasca**, A. Diaspro and S. Giordani, Beilstein J. Nanotechnol. 2017, 8, 1878–1888; doi:10.3762/bjnano.8.188.
6. "Photocatalytic Initiation of Radical Thiol–ene Reactions Using Carbon-Bi₂O₃Nanocomposites", V. Maffei, R. O McCourt, R. Petracca, O. Laethem, **A. Camisasca**, P. E Colavita, S. Giordani, Eoin M Scanlan, ACS Applied Nano Materials 1 (8), 4120-4126; DOI: 10.1021/acsanm.8b00870.

7. "Carbon Nano-Onions for Bioimaging and Cancer Therapy applications", **A. Camisasca**, S. Giordani, Book chapter in: Gonçalves G., Tobias G. (eds) *Nanooncology*, pp 417-455. Nanomedicine and Nanotoxicology. Springer, Cham (2018).

Communications at Conferences

Oral communications:

1. **A. Camisasca**, J. Bartelmess, S. Giordani "Fluorophore functionalized carbon nano-onions for NIR imaging" 10th E-WISPOC, Bressanone, Italy, 31 January-5 February 2016.
2. **A. Camisasca**, S. Lettieri, Marta d'Amora, S. Giordani "NIR fluorescent carbon nano-onions for cellular imaging", 27th International Conference on Diamond and Carbon Materials, Montpellier, France, 4-8 September 2016.
3. **A. Camisasca**, S. Lettieri, M. d'Amora, S. Giordani "Far-red fluorescent carbon nano-onions for high-resolution cellular imaging", Applied Nanotechnology and Nanoscience International Conference – ANNIC 2017, Rome, Italy, 18-20 October 2017.
4. **A. Camisasca**, A. Sacco, R. Brescia, S. Giordani "Boron/nitrogen co-doped carbon nano-onions as efficient and durable electrocatalysts for oxygen reduction reaction " PhotoIUPAC 2018, Dublin, Ireland, 8-13 July 2018.
5. **A. Camisasca**, A. Sacco, R. Brescia, S. Giordani "Boron/nitrogen co-doped carbon nano-onions as promising electrocatalyst for oxygen reduction reaction" NanoteC18, Brighton, UK, 29 August - 1 September 2018.

Poster communications

1. **A. Camisasca**, J. Bartelmess, S. Giordani "Fluorophore functionalized carbon nano-onions for NIR imaging" 10th E-WISPOC, Bressanone, January 31- February 5 2016.
2. **A. Camisasca**, S. Lettieri, M. d'Amora, A. Diaspro, T. Uchida, Y. Nakajima, K. Yanagisawa, T. Maekawa, S. Giordani "Far-Red Fluorescent Carbon Nano-Onions As Biocompatible Platform For Cellular Imaging", NanoteC17, Nantes, France, August 30 – September 2 2017.

Congresses Attended

1. 27th International Conference on Diamond and Carbon Materials, Montpellier, France. 4-8 September 2016.
2. NanoteC17, Nantes, France, August 30 – September 2 2017.
3. Applied Nanotechnology and Nanoscience International Conference – ANNIC 2017, Rome, Italy, 18-20 October 2017.
4. PhotoIUPAC 2018, Dublin, Ireland, 8-13 July 2018.
5. NanoteC18, Brighton, UK, 29 August –1 September 2018.

Courseware

Courses attended and passed

General Courses: B-type *Courses Given by Teachers of the IIT*

- 1. Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations (7 hours)**
Taught by: Luca de Trizio
Credits: 1
- 2. Basics of Crystallography and Diffraction by crystals (7 hours)**
Taught by: Mirko Prato
Credits: 1
- 3. Introductory course on transmission electron microscopy**
Taught by:: Rosaria Brescia, Zhiya Dang, Joka Buha, Roberto Marotta
Credits: 1
- 4. Opto-Electronic Properties of Semiconductor Quantum Dots**
Taught by: Iwan Moreel
Credits: 1
- 5. Science and Technology of 2D Crystals**
Taught by: Francesco Bonaccorso
Credits: 1
- 6. Magnetic properties and characterization techniques**
Taught by: Aidin Lak
Credits: 1
- 7. Spectroscopies for chemical analysis**
Taught by: Francisco Palazon, Roman Krahne, Sandeep Ghosh
Credits: 1
- 8. Application of Nanocrystals in energy storage, photo-catalysis and heterogeneous catalysis (7 hours)**
Taught by:: Massimo Colombo, Dipak Shinde, Simone Monaco
Credits: 1

General Courses: *B-type Courses activated by the University of Genova*

1. Electronic properties of solids

Taught by: Liberato Manna

Credits: 3

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

1. "Medicinal chemistry with carbohydrates: the influenza virus and the discovery of sialidase inhibitors" at Unige, Genoa, Italy; 13/11/2015, Speaker: Prof. Anna Berardi, Università di Milano.
2. "Low and Very Low Temperatures: Methods of Producing and Measuring Cryogenic Temperatures" at Unige, Genoa, Italy; 17/02/2016 – 18/02/2016, Speaker: Ivan Curlic, Department of Physics, Mathematics and Techniques, University of Prešov, Slovakia.
3. "NIR spectroscopy: theory and applications" at Unige, Genoa, Italy; 29/02/2016, Speaker: Dr. Tiziana Cattaneo and Dr. Roberto Giangiacomo, CRA-IIA, Milano, Italy.

4. "Magnetic hyperthermia: from fundamentals to biomedical applications" at the IIT, 05/05/2016 – 06/05/2016, Speaker: Dr. Francisco Terán, iMdea Nanociencia, Ciudad Universitaria de Cantoblanco, Madrid, Spain.
5. "Functional chromophores – syntheses and applications" at Unige, Genoa, Italy; 09/06/2016 – 10/06/2016. Speaker: Prof. Thomas J.J. Muller, Heinrich Heine Universität, Düsseldorf, Germany.

National and International Schools or Workshops

1. 10th E-WISPOC, Bressanone, Italy, 31 January-5 February 2016.

Seminars

1. Control of surface chemistry of nanodiamonds for bio-applications, Jean-Charles Arnauld; 09/11/2015
2. Semiconductor Nanocrystals: Discovery, Milestones, and Recent Theoretical Developments, Alexander L. Efros, Naval Research Laboratory, Washington, DC; 20/11/2015
3. Synthesis and Chemical Manipulation of Nanoparticles for a Magnetic Improvement, Veronica Salguero; 11/12/2015
4. Natural Polymers Of Bacterial Origin And Their Medical Applications, Ipsita Roy; 18/12/2015
5. Recent Advances With FIB-milled Microcavities, Lucas Flatten; 19/01/2016
6. Ribosomes: a spectacular prebiotic machine, Ada Yonath; 15/02/2016
7. Network Of Neurons and Carbon Nanotubes: Interfacing Neuronal Growth And Function, Laura Ballerini; 25/02/2016
8. Spatio-temporal visualization of atomic motions in low-dimensional materials, Giovanni Maria Vanacore; 03/05/2016
9. First-principle predictions of substrate effect on silicone, Udo Schwingenschloegl; 09/05/2016
10. Ionic bonding and the effect of electron repulsion on the band structure, Liberato Manna; 08/06/2016
11. Diversity oriented synthesis of functional dyes – novel sequences, novel structures, novel properties, Thomas J.J. Muller; 09/06/2016
12. Combined Light Harvesting and Charge Transfer in Complex Macromolecular Architectures, Amy M. Scott; 14/06/2016
13. Halocarbons in Nanomedicine and Nanotechnology: New Opportunities and Challenges, Pierangelo Metrangolo; 07/10/2016
14. Thermal Forces: Moving and Manipulating Matter With Thermal Gradients, Roberto Piazza; 21/10/2016
15. From cancer biology to drug treatment: Oxaliplatin in the era of personalized medicine, Paola Perego; 28/02/2017
16. Structural biopolymers – using Nature's building blocks as an inspiration for advanced manufacturing, Benedetto Marelli; 01/03/2017
17. Theatrocracy: the communication in the modern age, Stefano Amoroso; 02/03/2017
18. Flexible electronics: materials, technology and applications, Teresa Emery; 26/05/2017
19. The Roadmap to Applications of Graphene and Related Materials, Andrea Ferrari; 29/05/2017

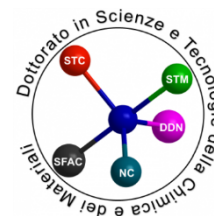
20. Carbon nanomaterials as imaging and diagnostic tools for nanomedicine, Silvia Giordani; 28/06/2017
21. Synthesis of nanostructures and materials via self-assembly and their application to biomedical studies, Toru Maekawa; 08/09/2017

Seminars Given

1. "Carbon nano-onions: promising biological imaging agents"; Seminar given at Bio-Nano Electronics Research Centre at Toyo University, Tokyo, Japan; 15/11/2016.
2. "Carbon nano-onions: a promising material for biological and electrochemical applications"; Seminar given at Dublin City University (DCU), Dublin, Ireland; 15/05/2018.
3. Monthly oral presentations at Nano Carbon Materials (NACM) group meeting; 2015-2018.



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



Curriculum: Chemical Sciences and Technologies

TULLIO CAVATTONI

Start of the Doctorate Program: *Novembre 1st 2015*
End of the Doctorate Program: *October 31st 2018*
Advisors: *Prof. Paola Riani, Prof. Fabio Canepa*

Thesis Title: Nanostructured Nickel- and Cobalt-based catalysts for producing useful compounds from renewables.

ACTIVITY REPORT
Research activity

Scientific Publications

Original publications on ISI Journals:

1. **Cavattoni T.**; Garbarino, G.; Catalytic abatement of biomass tar: a technological perspective of Ni-based catalysts, *Rendiconti Lincei* 2017, **28**; 68-85;
2. Garbarino G., Wang C., **Cavattoni T.**, Finocchio E., Riani P., Flytzani-Stephanopoulos M., Busca G.: A study of Ni/La-Al₂O₃ catalysts: a competitive system for CO₂ Methanation; submitted to *Applied Catal. B*
3. Garbarino G., **Cavattoni T.**, Riani P., Brescia R., Canepa F., Busca G.: Nickel-Cobalt alloy nanoparticles: effect of preparation procedure in the catalytic activity in ethanol steam reforming; submitted to *Molecular Catalysis*.
4. **Cavattoni T.**, Garbarino G., Riani P., Busca G.: Deactivation and selectivity switches during CO₂ methanation and Ethanol Steam reforming over Co/SiO₂ catalysts; to be submitted to *Applied Catalysis A General*
5. Garbarino G., Pugliese F., **Cavattoni T.**, Riani P., Busca G., Costamagna P.: Methane steam reforming and CO₂ methanation over commercial nickel/calcium aluminate catalysts: experimental study
6. Experimental study and laboratory reactor modelling; in preparation, to be submitted to *Chemical Engineering Journal*

Communications at Conferences

Poster Communications:

1. Co/SiO₂ based catalysts: effect of preparation procedure on catalytic activity in ethanol steam reforming and CO₂ methanation. G. Garbarino, **T. Cavattoni**, P. Riani, G. Busca; XI INSTM Conference, Luglio 12-15 2017, Ischia (NA)
2. Metal based nanoparticles as heterogeneous catalysts, **T. Cavattoni**, G. Garbarino, F. Canepa, G. Busca, P. Riani, "Programma PhD: La formazione post lauream e il mondo del lavoro - Nell'Industria Chimica, chi fa Ricerca... fa Carriera?" Workshop FEDERCHIMICA, 24 Maggio 2017, Genova
3. Co and Ni Mono- and bimetallic nanoparticles for catalysis applications, **T. Cavattoni**, G. Garbarino, R. Brescia, P. Riani, F. Canepa, G. Busca; Europacat, 13° European Congress on Catalysis, 27-31 Agosto 2017, Firenze
4. Methane Steam Reforming and CO₂ methanation over commercial Nickel/Calcium Aluminate catalysts: experimental study and laboratory reactor modelling, G. Garbarino, F. Pugliese, **T. Cavattoni**, P. Riani, G. Busca, P. Costamagna; International Conference on Chemical Reaction Engineering, P263, Firenze 20-23 Maggio 2018

Oral Communications:

1. Mono- and bimetallic nanoparticles as catalysts in ethanol steam reforming, **T. Cavattoni**, G. Garbarino, G. Busca, F. Canepa, P. Riani, Giornata della Chimica Ligure 2017: Le attuali tendenze della ricerca chimica in Liguria, 20 ottobre 2017, Genova.
2. Co and (Co, Ni) Nanoparticles: effect of preparation procedure on catalytic activity in ethanol steam reforming and CO₂ methanation; G. Garbarino, **T. Cavattoni**, F. Canepa, Brescia R., G. Busca, P. Riani; XI INSTM Conference, Luglio 12-15 2017, Ischia (NA)

Courseware

Courses attended and passed

1. "Struttura elettronica nei solidi" (Trattazione Elementare), L. Manna (IIT) (3 credits)
2. "Nanoparticle characterization by atomic force microscopy and dynamic light scattering", Ranieri Rolandi (DIFI) (2 credits)
3. Catalizzatori ed Adsorbenti industriali, G. Busca (DICCA) (2 credits)
4. "Fondamenti di Fondamenti di microscopia elettronica a scansione ed in trasmissione", Paola Riani DCCI (3 credits)
5. Perspectives on bioinorganic chemistry, S. de Negri (DCCI) (2 credits)

Courses given by invited experts:

1. "NIR spectroscopy: theory and applications" dr. Tiziana Cattaneo e dr. Roberto Giangiacomo(CRA-IAA Consiglio per la Ricerca in agricoltura e l'analisi dell'economia agraria) Unità di ricerca per i processi dell'industria agro-alimentare Ingegneria e Trasformazioni agroalimentari, Milano), Genova 29/02/2016
2. "Magnetic hyperthermia: from fundamentals to biomedical applications" Dr. Francisco Terán (iMdea Nanociencia, Ciudad Universitaria de Cantoblanco/Nanobiotecnologia, CNB-CSIC-iMdea Nanociencia, Campus Universitario de Campoblanco, Madrid, Spain) IIT Genova 05-06/05/2016

3. "Advanced materials for Renewable Energy (Energy I Saving)" Prof. Peter Rogl (Institute of Physical Chemistry, University of Vienna, Austria) 14 e 16/06/2016 DCCI Genova
4. "Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials – Novel Materials for energy storage and conversion" Prof. Dr. Thomas Fässler (Department of Chemistry – Technical University of Munich, Germany) 11/05/2017 DCCI
5. "Approaches to synthesis and characterization of magnetic nanomaterials for biomedical applications" Dott. Davide Peddis (Istituto di Struttura della Materia, CNR-Roma) 23-24/01/2018, DCCI Genova.

National and International Schools or Workshops

1. Elitecat 2017, Summer School, Lione-Villeurbanne, France, 3-7/07/2017
2. Catalysis Fundamentals and Practice, Summer School, Liverpool, U.K., 17-21/07/2017
3. Young Researchers Winter School, Padova, 22/02/2017

Seminars Attended

1. "Self-assembly of Magnetic Nanomaterials: Design and Physical Properties" C.Petit 13/06/2016
2. "Refinery, green refinery and biofuel: today and tomorrow." C. Perego 20/01/2017, DICCA
3. "Designing oxidation, reduction and multifunctional green catalysts" Prof. Avelino Corma (Polytechnic University of Valencia) 23/02/2017
4. "Development of novel non-critical metal catalysts to catalyze the transformation of lignocellulosic waste into renewable industrial feedstocks" Prof. Graham J. Hutchings (Cardiff University) 23/02/2017
5. "Smart biomass conversion with non-critical metal/metal-oxide catalysts" Dr. K. Nakajima (Hokkaido University) 23/02/2017
6. "Understanding catalysts under fluctuating reaction conditions" Prof. Jan-Dierk Grunwaldt (Karlsruhe Institute of Technology) 23/02/2017
7. "Structure unit-based design of complex metal oxide catalysts for biomass conversion" Prof. Wataru Ueda (Kanagawa University) 23/02/2017
8. "Structured Materials from Polymer Colloids" M.Morbidelli, 05/05/2017 DICCA (*firma di presenza non disponibile in quanto foglio firme non presente*)
9. "Programma PhD: La formazione post lauream e il mondo del lavoro - Nell'Industria Chimica, chi fa Ricerca... fa Carriera?" 24/05/2017, Genova
10. "Atomic Structure and mass-production of size-selected nanoparticles (clusters)", R.E. Palmer 30/05/2017, DIFI (*firma di presenza non disponibile in quanto foglio firme non presente*)
11. "Analisi termica accoppiata alla gas cromatografia e spettrometria di massa. Un potente strumento per la caratterizzazioni dei materiali" F. Locardi, 13/06/2017 DCCI
12. "Il contributo del DCCI al Programma Nazionale di Ricerche in Antartide" Prof. Mario Grotti – Prof.ssa Paola Rivaro, 27/02/2018
13. "Control and Diagnosis of Fuel Cells, from Research to Design", Prof. Cesare Pianesse (Universita degli studi di Salerno) 20/04/2018
14. "Epigenetic changes, trace elements and antioxidant status for cancer prevention" Prof.ssa Barbara Anna Bobtowska-Korczak, 24/05/2018

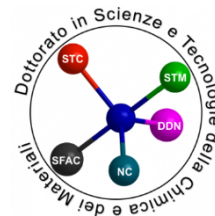
15. "Targeting the purinergic signaling in the heart. New perspectives for understanding the electrophysiological role of adenosine in atrial fibrillation" Dr. Luca Soattin (PhD candidate Cardiac Physiology Laboratory - Københavns Universitet), 04/06/2018
16. "Designing and Studying Perovskite Materials for a Renewable Energy Future", Prof. Clemens Burda 06/06/2018.

OtherActivities

1. Attività di supporto alla didattica relative all'insegnamento Chimica Generale ed Inorganica con Laboratorio, 15/11/2016 - 10/01/2017, per un totale di 24 ore.
2. Attività di supporto alla didattica relativa al lavoro di tesi di laurea triennale in Ingegneria Chimica degli studenti Giulia Piazza e Beatrice Antonucci, Aprile 2017 – Settembre 2017



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



Curriculum: Chemical Sciences and Technologies

SEIF EDDINE FENNI

PhD. In **Co-tutoring program** between
the University of FERHAT Abbes Setif-1 (Algeria) and the University of GENOVA .

Start of the Doctorate Program: *November 1st, 2015*

End of the Doctorate Program: *October 31st, 2018*

Advisors: Prof. Dario Cavallo, Prof. Nacereddine Haddaoui

Thesis Title: Crystallization of poly(lactide) in multiphasic polymer blends and composite

Thesis abstract

The work of thesis is focused on studying the crystallization behavior of polymer blends and composite based on poly(L-lactide) (PLLA). Different multiphasic systems will be studied, with the aim of improving PLLA crystallization kinetics and mechanical properties (i.e., reducing the PLLA brittleness). As such, the preparation of the novel material and the effect of the addition of other polymers, immiscible with PLLA, or solid phase (nanoparticles) will be studied.

As an example, in the first two years of PhD we studied blends of poly(butylene succinate) (PBS) and PLLA in the presence of graphene oxide nanosheets (GO). It has been shown that GO improve the adhesion between PLLA and PBS and act as a nucleating agent for for both semi-crystalline polymers, with more pronounced nucleating efficiency for the PBS phase.

In the second year, PLLA/PU immiscible blends were studied. Blends were prepared by melt blending in an internal mixer (Brabender). Mechanical properties showed that occurrence of dynamic vulcanization (of PLLA, glycerol and hydroxyl-terminated fatty acid polyesters) and formation of PU network inside PLLA leads to large enhancement in the impact strength of the material. Thermal characterization showed a slight decrease in the thermal stability of PLLA, followed by a decrease in crystallizability of the PLLA component. However, the presence of PU phase dispersed within the PLLA matrix resulted in a faster nucleation process.

In the last year, we studied the morphology, nucleation, and crystallization behavior of binary and ternary blends based on triple-crystalline polymers (PLLA, PBS and polycaprolactone (PCL)). Morphological analysis revealed the occurrence of sea-island morphology in all the binary blends, while a "partial wetting" morphology was observed in all ternary blends in which the

minor phase is located at the interface between the two major components. DSC analysis showed the presence of coincident crystallization and fractionated crystallization in different blends, while no nucleation or enhancement in the crystallization rate was observed notwithstanding the composition. Polarized optical microscopy (POM) analysis revealed an interface-induced nucleation phenomenon, i.e., PLA nucleates on both molten PCL and PBS droplets (with higher nucleation ability of molten PCL with respect to molten PBS). Moreover, the PBS phase was found to nucleate on the previously crystallized PLA in the PLA/PCL/PBS: 45/10/45 wt% blend.

ACTIVITY REPORT

Research Activity

The research activity was mainly carried out at the DCCI in Genova, with some work in the University of Setif-1 in Algeria, CNR-ISMAR (Genova), and the University of the Basque country (Spain).

Scientific Publications

1. **S.E. Fenni**, O. Monticelli, L. Conzatti, R. Doufnoune, P. Stagnaro, N. Haddaoui, D. Cavallo: "Correlating the morphology of poly(l-lactide)/poly(butylene succinate)/graphene oxide blends nanocomposites with their crystallization behavior" accepted on eXPRESS Polymer Letters. Vol 12 (2018) 58-70.
2. **S.E. Fenni**, D. Cavallo, A.J Müller: "Nucleation and crystallization in bio-based immiscible polyester blends". Book chapter in: Editor: Di Lorenzo ML, Androsch R (eds) Advances in Polymer Sciences: Thermal Properties of Bio-based Polymers. Springer, submitted.
3. **S.E. Fenni**, O. Monticelli, D. Cavallo, N. Haddaoui: "Renewable and super-toughened poly (L-lactic acid)/polyurethane blend prepared by dynamic vulcanization". In preparation.
4. **S.E. Fenni**, N. Haddaoui, B.D. Favis, A.J Müller, D. Cavallo: "Morphology and crystallization behavior of binary and ternary blends based on PLA, PCL, and PBS". In preparation.

Communications at Conferences

Poster Communications:

1. **S.E. Fenni**, D. Cavallo and N. Haddaoui: Morphology and thermal properties of poly(l-lactide)/poly(butylene succinate) bioblend nanocomposites with graphene oxide nano-sheets. Conférence Internationale sur les Matériaux Polymères et leurs Composites « CIMPC'17 » (25 – 27 April 2017, University of Tlemcen - Algeria).
2. **S.E. Fenni**, D. Cavallo and N. Haddaoui: Study of the system nanocomposite Bio-blend PLLA / PBS using GO nanofiller: Compatibilization and crystallization behavior. Ph.D. student Day, (10 Mai 2017 University of Ferhat Abbas Setif-1 – Algeria).
3. **S.E. Fenni**, N. Haddaoui and D. Cavallo: Relations between morphology and crystallization behavior of poly(l-lactide)/poly(butylene succinate) bioblend nanocomposites with graphene oxide nano-sheets. International Discussion Meeting on Polymer Crystallization 2017 «IDMPC 2017» (17 – 20 September 2017, Martin Luther University Halle-Wittenberg – Germany).

4. **S.E. Fenni**, D. Cavallo and N. Haddaoui: Thermal analysis and crystallization behavior of poly(l-lactide)/poly(butylene succinate) / graphene oxide blend nanocomposites. 13th Mediterranean Conference on Calorimetry and Thermal Analysis «Medicta 2017» (24 - 27 September 2017, Loano – Italy).
5. **S.E. Fenni**, N. Haddaoui and D. Cavallo: Dynamic vulcanization of polyester polyol in polylactide matrix as an effective way for PLA toughening. Ph.D. student Day, (02 May 2018 University of Ferhat Abbes Setif-1 – Algeria).

Courseware

B-type Courses:

1. Transitions and Relaxations in Amorphous and Semi crystalline Organic Polymers and Copolymers, presented by prof. N. Haddaoui from the UFAS-1. 23 April – 11 Mai 2017, Process Engineering Department, University of Ferhat Abbes Setif-1 (UFAS-1) (Algeria): (3 credits).
2. Multivariate analysis of chemical data, presented by M. Casale, R. Leardi and P. Olivieri. DIFAR-University of Genoa: (3 credits).
3. Introduzione all'applicazione della spettroscopia RAMAN ai materiali, presented by M. M. Carnasciali, DCCI (2 credits)
4. Experimental design, presented by Prof Riccardo Leardi, Department of Economy, Genoa. (4 credits).

A-type Courses:

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

Seminars Attended:

1. Vincenzo Buscaglia from ICMATE-CNR, "Synthesis of high permittivity nanoparticles by hydrothermal and solvothermal methods" (29th March 2017 in CNR – Genoa).
2. Paola Stagnaro from ISMAC-CNR, "Polymer-based Composites: Process-Structure Properties Relationship" (29th March 2017 in CNR – Genoa).
3. Leontin Padurariu from "Al I. Cuza" University, Romania, "3D Finite Element Method modelling of dielectric and ferroelectric properties of composite systems" (29th March 2017 in CNR – Genoa).
4. Lavinia Curecheriu from "Al I. Cuza" University, Romania, "Electrical properties of chitosan-based composites: Towards active dielectrics for flexible electronics" (29th March 2017 in CNR – Genoa).
5. Davide Comoretto from DCCI - UNIGE, "All-Polymer Nano-Photonics: from Lasers to Sensors" (29th March 2017 in CNR – Genoa).
6. L. Zerroual from UFAS-1, towards a new technology of lead acid batteries (10th May 2017 in University of Setif -1, Algeria).

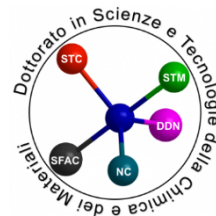
7. T. Aissaoui from UFAS-1, Essential steps for Algerian researcher to target ISI journals (10th Mai 2017 in University of Setif -1, Algeria).
8. Richard E. Palmer from University of Birmingham, "Atomic structure and mass-production of size-selected nanoparticles (clusters)" (30th Mai 2017, DIFI – Genoa).
9. S. Riva from CNR – Milano, "Un caso di proficua collaborazione: biocatalisi e prodotti naturali" (16th June 2017, DCCI – Genoa).
10. Jason K. Sello from Brown University of Providence (USA), "Novel small molecules, targets, and strategies in anti-infective development" (3th July 2017, DCCI – Genoa).
11. Julian Sereni from Instituto Balseiro Centro Atomico Bariloche (Argentina), "Cryocooler materials for Adiabatic Demagnetization: Comparison between paramagnetic salts and intermetallic compounds" (4th July 2017, DCCI – Genoa).
12. Paolo Mele from Muroran Institute of Technology, Hokkaido (Japan), "On research activities at Muroran Institute of Technology" (24th July 2017, DCCI – Genoa).
13. Nevena Marinova from the University of the Basque country (Spain), "Light and oxygen resistant methyl ammonium lead iodide perovskite stabilized with hindered amine light stabilizer" (23rd February 2018, Auditorium Korta – San Sebastian, Spain).
14. Nadia Lotti from the University of the Bologna (Italy), "New biobased polyesters: structure-property relationship" (09th March 2018, Physics Department – San Sebastian, Spain).
15. Ulrich S. Schubert from Friedrich-Schiller-University Jena (Germany), "Polymers for batteries" (11th Mai 2018, Auditorium Korta – San Sebastian, Spain).
16. Thomas Thurn-Albrecht from the University of Halle-Wittenberg (Germany), "Microscopic Observation of Interface-Induced Crystallization via Prefreezing in Polymers Melts" (16th June 2018, Auditorium Korta – San Sebastian, Spain).

National and International Schools or Workshops:

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



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



Curriculum: Chemical Sciences and Technologies

AURELIO FERRUCCI

Start of the Doctorate Program: *November 1st, 2015*

End of the Doctorate Program: *October 31st, 2018*

Advisor: Prof. Vincenzo Dovì

Thesis Title: Innovative strategies to optimize water resources

Thesis abstract

The research project is aimed to highlight an overall strategy to optimize the use of water resources in industrial environment and in the environments enlarged to the surrounding territory (total site integration)

For this purpose the study will focus on a specific industrial systems characterized by relevant economic costs due to water streams distribution, regeneration and reuse and by the need of respecting at the same time diverse contaminants concentration constraints for the various production processes involved.

There are various aspects which must be analysed while carrying out this work, whose relevance (and therefore the related contribution during the development of the research work) will depend on the particular structure of the considered system.

1. Identification and reconciliation of process data applying innovative algorithms able to manage heteroscedasticity and censored data.
2. Preliminary process stream configuration study based on water pinch analysis.
3. Techno – economic evaluation – based on water pinch analysis results - of the techniques and the degree of decontamination of the water streams undergoing regeneration treatments.
4. Sensitivity analysis to highlight the overriding interventions.
5. Rigorous mathematical modelling of the final arrangement of water and steam streams and of the regeneration process units to highlight the optimal treatment configuration.

ACTIVITY REPORT

Research Activity

The research activity was mainly carried out at the DCCI

Scientific Publications

Original publications on ISI Journals:

1. **Ferrucci, A.**, Vocciante, M., Bagatin, R., and Ferro, S. 2017. *Electrokinetic remediation of soils contaminated by potentially toxic metals: Dedicated analytical tools for assessing the contamination baseline in a complex scenario*. Journal of Environmental Management 203: 1163-1168.
2. Vocciante, M., De Folly D'Auris, A., Finocchi, A., Tagliabue, M., Bellettato, M., **Ferrucci, A.**, Reverberi, A.P., and Ferro, S. 2018. *Adsorption of ammonium on clinoptilolite in presence of competing cations: Investigation on groundwater remediation*. Journal of Cleaner Production 198: 480-487.
3. **Ferrucci, A.**, Reverberi, A.P., Dovì, V.G., and Vocciante, M. 2018. *Including Fluctuations of Water Content in Feed Streams and Products for the Optimal Management of Water Resources*. Chemical Engineering Transactions 70: 1123-1128.

Communications at Conferences

Oral communications:

1. 11th Sdewes Conference – Lisbon September 2016 – “*Electrokinetic remediation of soils polluted by heavy metals: dedicated analytical tools for assessing the contamination baseline in a complex scenario*”
2. 16th International Downstream Technology and Strategy Conference – Madrid May 2016 – “*What is the added value brought by a reliable refinery planning-scheduling solution?*”
3. 2nd Indonesia Refining and Petrochemical Convention 2016 – Jakarta – October 2016 – “*Use smart LP tools to support the development of refinery configuration studies*”
4. Refining & Petrochemical World China 2016 – Beijing November 2016 – “*What is the added value brought by a reliable refinery planning-scheduling solution?*”
5. 12th sdewes Conference – Dubrovnik October 2017 – “*Competitive Adsorption of Ammonium on Zeolites: Investigation for Applications in Groundwater Remediation*”
6. CHISA 2018 and PRES 2018 Conference – Prague August 2018 – “*Including Fluctuations of Water Content in Feed Streams and Products for the Optimal Management of Water Resources*” (Poster session)

Congresses Attended

1. 11th sdewes Conference – Lisbon September 2016.
2. 16th International Downstream Technology and Strategy Conference – Madrid May 2016.
3. 2nd Indonesia Refining and Petrochemical Convention 2016 – Jakarta – October 2016.
4. Refining & Petrochemical World China 2016 – Beijing November
5. 12th sdewes Conference – Dubrovnik October 2017.

6. CHISA 2018 and PRES 2018 Conference – Prague August 2018.

Courseware

Courses attended and passed:

1. Multivariate analysis of chemical data (3 credits).
2. Experimental Design (3 credits).
3. Process Intensification (3 credits).
4. Mathematical Methods For Chemistry (2 credits)

Courses Given by invited experts:

1. *New methods for food safety and authenticity testing* – Valeria Merlo – DCCI – November 27th 2015
2. *Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials* – Prof. Dr. Thomas F. Fassler – DCCI – May 11th 2017
3. *Novel Materials for energy storage and conversion*– Prof. Dr. Thomas F. Fassler – DCCI – May 11th 2017
4. *Superhard Materials: Structural Chemistry of Boron and Borides* – Prof. PETER ROGL – June 6th,7th 2017

National and International Schools or Workshops

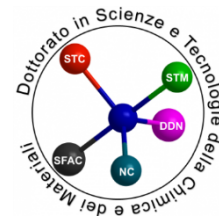
1. IWIW 2016 International Workshop on industrial waste (DCCI Genova). 1 day
2. Chemometric Tools for Process Monitoring School (UNIMORE Modena February 2018) 3 days.
3. School of Experimental Design (DIFAR Genova, June 2018) 4 days.
4. School of Multivariate Analysis (DIFAR Genova, September 2018) 4 days.

Seminars Attended

1. NIR spectroscopy: theory and applications – Tiziana Cattaneo, Roberto Giangiacomo – DIFAR – February 29th 2016
2. *Aspetti e prospettive della moderna industria siderurgica* – Franco Belgrano – DCCI – May 5th 2016



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



Curriculum: Chemical Sciences and Technologies

RICCARDO FRECCERO

Start of the Doctorate Program: November 1st, 2015

End of the Doctorate Program: October 31st, 2018

Advisors: Prof. Adriana Saccone, Dr. Frank R. Wagner

Thesis Title: Study of new polar intermetallic compounds: synthesis, structural relations and real space chemical bonding analysis

Thesis abstract

The study of binary, ternary and multicomponent intermetallic compounds is of great interest for solid-state inorganic chemistry. In particular, the interplays between composition, crystal structure and physical properties are far to be completely understood. These lacks are mainly due to the poor knowledge of chemical bonding establishing among the constituting elements of intermetallic compounds. Thus, a systematic research, both experimental and theoretical, will be carried out focusing on Zintl and polar intermetallics, which show structural and chemical bonding peculiarities together with intriguing physical properties, representing excellent candidates to give insight into the aforementioned relations. Hence, a systematical study both on binary $R\text{-Ge}$ and ternary $R\text{-M-Ge}$ tetrelides (R = rare earth metal; M = another metal) will be conducted. In particular the $R_2M\text{Ge}_6$ family of intermetallic compounds, where polyanionic networks of $(2b)\text{Ge}^{2-}$ and $(3b)\text{Ge}^-$ occurs, has been selected as the starting point for this project. Compounds where the M metal is expected to behave as a cation (M = Li, Mg, Al, Zn) will be investigated, moving then to more complex and unusual scenarios where the M metals act as anions (M = Pd). Synthesis both with traditional and innovative methods, i.e. metal flux synthesis, will be performed. Phases will be characterized by means of LOM, SEM-EDXS, powder X-ray diffraction, DTA and DSC. Crystal structure of synthesized compounds will be deduced from X-ray single crystal data and subsequently used to perform chemical bonding analysis mainly applying new direct-space techniques, such as QTAIM (Quantum Theory of Atoms In Molecules) and ELI-D (Electron Localizability Indicator).

ACTIVITY REPORT

Research Activity

Research Period Abroad

1. Research period (**4 months**) at the Max Plank Institute for Chemical Physics of Solids (Dresden, Germany) related to my PhD thesis; 10/03/2017-31/01/2018
2. **2 weeks** at the Max Plank Institute for Chemical Physics of Solids (Dresden, Germany) to discuss on the topic "Chemical bonding in R_2MGe_6 compounds" (R= rare earth metal; M= Li, Mg, Al, Zn, Pd, Cu, Ag); 09/17/2018-09/28/2018
3. **7 days** at the Max Plank Institute for Chemical Physics of Solids (Dresden, Germany) to attend the ChemBond conference and to discuss obtained results for chemical bonding in R_2MGe_6 (R= rare earth metal; M= Mg, Zn) compounds; 11/27/2016-12/3/2016

Research Projects

1. Italian SuperComputing Resource Allocation – (ISCRA Award -Class C, 150000 h/cpu) from CINECA for the project "Y-NiMS" (Yttrium Nickel Magnesium System) HP10CAINNP (PI); 06/08/2018 – 03/08/2019

Scientific Publications

Original publications on ISI Journals:

1. **R. Freccero**, P. Solokha, S. De Negri, A. Saccone, Yu. Grin, F.R. Wagner, "Analysis of polar-covalent bonding beyond the Zintl picture in intermetallic germanides La_2MGe_6 , M = Li, Mg, Al, Zn, Cu, Ag, Pd and Y_2PdGe_6 ", Chem. Eur. J., Submitted 2018
2. **R. Freccero**, S.H. Choi, P. Solokha, S. De Negri, T. Takeuchi, S. Hirai, P. Mele, A. Saccone, "Synthesis, crystal structure and physical properties of $Yb_2Pd_3Ge_5$ " J. Alloys Compd., Submitted 2018
3. **R. Freccero**, P. Solokha, D. M. Proserpio, A. Saccone, S. De Negri, "Lu₅Pd₄Ge₈ and Lu₃Pd₄Ge₄: Two More Germanides among Polar Intermetallics", Crystals, 2018, 8 (5), 205 DOI: 10.3390/cryst8050205
4. **R. Freccero**, P. Solokha, D. M. Proserpio, A. Saccone, S. De Negri, "A new glance on the R_2MGe_6 (R = rare earth metal, M = another metal) compounds. An experimental and theoretical study of R_2PdGe_6 germanides", Dalton Trans., 2017, 46, 14021-14033 DOI: 10.1039/C7DT02686B
5. P. Solokha, **R. Freccero**, S. De Negri, D. M. Proserpio, A. Saccone; "The $R_2Pd_3Ge_5$ (R = La–Nd, Sm) germanides: synthesis, crystal structure and symmetry reduction" Struct Chem, 2016, 27, 1693–1701 DOI:10.1007/s11224-016-0812-z

Communications at Conferences

Oral communications:

1. **R. Freccero**, F.R. Wagner, P. Solokha, S. De Negri, J. Grin, A. Saccone, "Comparative real space chemical bonding analysis of La_2MGe_6 (M = Li, Mg, Al) intermetallics"; proceedings of the "XLVI Congresso Nazionale di Chimica Inorganica", Bologna (Italy), 09/10-09/13/2018, OC56, pag 83.
2. **R. Freccero**, F.R. Wagner, P. Solokha, S. De Negri, Yu. Grin, A. Saccone; "Chemical bonding scenarios bridging intermetallics to coordination compounds: the La_2MGe_6 (M = Mg, Zn)

germanides case study”; proceedings of the “XLIV Congresso Nazionale di Chimica Inorganica”, Padova (Italy), 09/14-09/17/2016, O57, pag. 73

Poster communications:

1. **R. Freccero**, P. Solokha, S. De Negri, A. Saccone; “The new Lu₃Pd₄Ge₄ intermetallic: the key role of thermal characterization on the road towards physical properties measurements”, proceedings of the “12th European Symposium on Thermal Analysis and Calorimetry (ESTAC12)”, 08/27-08/30/2018, Brasov – Romania, Poster PS1.032, pag. 216
2. **R. Freccero**, P. Solokha, Davide M. proserpio, A. Saccone, S. De Negri; “Two novel polar intermetallics Lu₅Pd₄Ge₈ and Lu₃Pd₄Ge₄: crystal structure and chemical bonding analysis”, proceedings of the “21st International Conference on Solid Compounds of Transition Elements-SCTE 2018”, 03/25-03/29/2018, Vienna – Austria, Poster Mo-PO22, pag. 25
3. **R. Freccero**, F.R. Wagner, P. Solokha, S. De Negri, Yu. Grin and A. Saccone; “Crystal structure and chemical bonding of La₂MGe₆ compounds (M = Mg/Zn)” proceedings of the “International Symposium on Material Design & the 11th USPEX Workshop”, Varenna (Lecco), 06/05-06/09/2016, pag. 18.

Congresses Attended

1. “XLVI Congresso Nazionale di Chimica Inorganica”, Bologna (Italy), 09/10-09/13/2018
2. “12th European Symposium on Thermal Analysis and Calorimetry (ESTAC12)”, 08/27-08/30/2018, Brasov (Romania)
3. “The 21st International Conference on Solid Compounds of Transition Elements-SCTE 2018”, 03/25-03/29/2018, Vienna (Austria)
4. “13th Mediterranean Conference on Calorimetry and Thermal Analysis – MEDICTA 2017”, 09/24-09/27/2017, Loano (SV)
5. Conference “Chemical bonding in Position Space (ChemBond2016)” at the Max Planck Institute for Chemical Physics of Solids, 11/27/2016 – /12/01/2016, Dresden (Germany)
6. “XLIV Congresso Nazionale di Chimica Inorganica”, Padova (Italy), 09/14-09/17/2016

Courseware

Courses attended and passed

Courses Given by Teachers of the Unige and IIT:

1. Mathematical Methods for Chemistry, Prof. Figari and prof. Rui, (2 credits)
2. Synthesis, structure and functional properties of intermetallic compounds, Prof. Saccone (2 credits)
3. Elementary electronic structure of solids Dr. Manna (3 credits)
4. Introduction to the RAMAN spectroscopy applied to materials Prof. Carnasciali (2 credits)
5. Principi di metallurgia applicata: tradizione ed innovazione Prof. Pinasco (2 credits)
6. The Rietveld method: fundamentals and applications Prof. Artini (2 credits)
7. Perspectives on bioinorganic chemistry Prof. De Negr (2 credits)

Courses Given by invited experts:

1. “The chemistry of metal borides and metal boron carbides”, prof. P. Rogl, 06/11-06/13/2018, DCCI, Genova
2. “From crystallography to imaging”, dr. C. Giannini, 04/23/2018 and 04/25/2018, IIT, Genova

3. "Superhard boron materials", prof. P. Rogl, DCCI, Genova
4. "Energy materials ", prof. T. Fassler, 05/11/2017, DCCI, Genova
5. "Advanced Materials for Renewable Energy (Energy I Saving)", Prof. Peter Rogl, 06/14/2016 and 06/16/2016, DCCI, Genova
6. "Low and Very Low Temperatures: Methods of Producing and Measuring Cryogenic Temperatures" Dr. Ivan Čurlík, 02/17-02/18/2016, DCCI, Genova
7. "New methods for food safety and authenticity testing", Dr. Merlo, 11/27/2015, DCCI, Genova
8. "Conventional and unconventional superconductivity-an overview", prof. Bauer, 11/09/2015 and 11/11/2015, DCCI, Genova

Seminars

1. Dr. Eteri Svanidze, "Micro-scale structuring of solid state systems" 20/09/2018, MPI CPfS, Dresden
2. Prof. P. Rivaro, prof. M. Grotti, "Il contributo del DCCI al programma nazionale di ricerca in Antartide", 02/27/2018, DCCI, Genova
3. Dr. Eteri Svanidze, "Novel on-centrosymmetric superconductor BeAu" 01/29/2018, MPI CPfS, Dresden
4. Dr. Manuel Feig, "Superconductivity of new Chevrel phases" 01/18/2018, MPI CPfS, Dresden
5. Dr. Oksana Matselko, "The Ga–Sn–Pd phase diagram" 01/11/2018, MPI CPfS, Dresden
6. Dr. Peter Höhn, "Structural complexity by 2-D intergrowth in Nitridomanganates" 12/11/2018, MPI CPfS, Dresden
7. Dr. Christina Birkel, "Synthesis and properties of selected 3D MAX phases and 2D MXenes" 11/27/2018, MPI CPfS, Dresden
8. Dr. William Clark, "High pressure synthesis and characterization of a novel iron nitride" 10/09/2018, MPI CPfS, Dresden
9. Dr. P Mele, "On research activities at Muroran Institute of Technologies", 07/24/2017, DCCI; Genova
10. Prof. Sereni, "Cryocooler materials for adiabatic demagnetization: comparaisn between paramagnetic salts and intermetallic compounds", 07/04/2017, DCCI, Genova

National and International Schools or Workshops

1. "Y-Rich 2017" workshop organized by the "Gruppo Giovani della Società Chimica Italiana", 06/23/2017, Rome
2. "Programma PhD – La formazione post lauream e il mondo del lavoro nell'industria Chimica, chi fa ricerca... Fa carriera?", 5° edition, 05/24/2017, Genova
3. DGrid (version 5.0) workshop, 12/01/2016, Dresden, Germany
4. "International symposium on material design & 11th USPEX workshop", Varenna (LECCO), 06/05-06/09/2016
5. "28th ad hoc workshop on Jana2006-Basics of Jana2006" at the "Department of structure analysis at the institute of physics", Prague (Czech Republic), 12/14-12/15/2015 (16 hours)

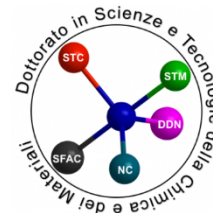
Other Activities

1. Acquisition of the 24 Formative University Credits (ECTS) in Psychology (6 CFU), Anthropology (6 CFU), Pedagogy (6 CFU) and Didactics Methodologies (6 CFU) necessary for the teaching abilitation in Italy; 02/2018 – 06/2018

2. Member of the organizing committee of the “13th Mediterranean Conference on Calorimetry and Thermal Analysis - MEDICTA 2017”, 24/09/2017 – 27/09/2017, Loano (SV).
3. Tutor (58h) for Chemistry and Chemical Technologies students attending the courses of “General and Inorganic Chemistry” and “Organic Chemistry 1”, at the Department of Chemistry and Industrial Chemistry of the Genoa University.
4. Teaching support for the course “Inorganic chemistry 1 with laboratory” (code: 65188) from March to May 2016 (30 hours)



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



Curriculum: Pharmaceutical, Food and Cosmetic Sciences

ILARIA GIACCHELLO

Start of the Doctorate Program: November 1st, 2015

End of the Doctorate Program: October 31st, 2018

Advisor: Prof. Grossi Giancarlo

Thesis Title: Synthesis of properly substituted pyridine and pyrimidine derivatives and their biological evaluation as potential antiviral agents

Thesis abstract

Viruses are aggregates of proteins and nucleic acids that are responsible for several human pathologies: among these, influenza or “flu” represents a serious worldwide health problem. Influenza viruses are a class of RNA viruses belonging to the *Orthomyxoviridae* family [1]. Nowadays, there are not many available antiviral drugs on the pharmaceutical market; for this reason the research in this field is very active.

My research doctorate project is based on the rational design and synthesis of molecules acting on RNA polymerase, a pivotal enzyme for RNA virus replication, that consists of three subunits: PA (polymerase acid protein), PB1 (polymerase basic protein 1) and PB2 (polymerase basic protein 2) [2]. According to the current scientific literature, the oblique interaction between PA carboxylic group and PB1 amine group is fundamental for virus replication, is maintained among several viral strains and involves few amino acids so that it could be inhibited by small molecules [3,4].

Molecular modeling studies carried out at the University of Perugia, showed that properly substituted pyridine and pyrimidine derivatives could inhibit PA-PB1 interaction. Starting from these computational studies, I synthesized a library of 3-cyanopyridine compounds 1, having in C2 a sulfanylacetamide chain ending with the methyl or benzyl ester of an L or D aminoacid, a library of pyrimidines 2 and some pyridine derivatives 3, both of them endowed with a 2-mercapto-*N*-(*m*-tolyl)acetamide chain and different aromatic substituent in C4 and/or C6 (Figure 1.). These derivatives were biologically evaluated in collaboration with the University of Padua, with, in some cases, good results [5].

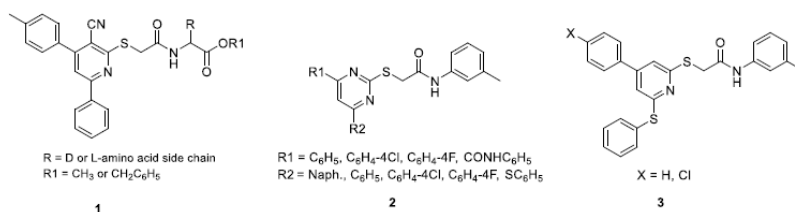


Figure 1. Structures of synthesized pyridine and pyrimidine derivatives 1, 2 and 3.

REFERENCES

- [1] <https://talk.ictvonline.org/>
- [2] Reich, S.; Guilligay, D.; Pflug, A., et al. *Nature* 516, 361-366 (2014).
- [3] He, X.; Zhou, J.; Bartlam, M., et al. *Nature* 454, 1123-1126 (2008).
- [4] Obayashi, E.; Yoshida H.; Kawai, F., et al. *Nature* 454, 1127-1131 (2008).
- [5] D'Agostino, I., Giacchello, I., Nannetti, G. et al. *Eur. J. Med. Chem.* 157, 743-758 (2018).

ACTIVITY REPORT

Research Activity

Research Period Abroad

Three month internship at the University of Basel, Department of Organic Chemistry, within the research group of Prof. Dr. Olivier Baudoin. 25/06/2018 – 23/09/2018.

Scientific Publications

1. D'Agostino, I., **Giacchello, I.**, Nannetti, G., Fallacara, A. L., Deodato, D., Musumeci, F., Grossi, G., Palù, G., Cau, Y. Trist, I. M., Loregian, A., Schenone, S., Botta, M. "Synthesis and biological evaluation of a library of hybrid derivatives as inhibitors of influenza virus PA-PB1 interaction". *European Journal of Medicinal Chemistry*, 157, 743-758 (2018).
2. Musumeci, F., Greco, C., **Giacchello, I.**, Fallacara, A. L., Ibrahim, M. M., Grossi, G., Brullo, C., Schenone, S. "An update on JAK inhibitors". *Current Medicinal Chemistry*, [e-pub ahead of print], (2018).
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 Opinion on Therapeutic Patents*, 1-14 (2017).

Communications at Conferences

Poster Communications:

1. **Giacchello, I.**, Trist, I. M. L., Musumeci, F., Greco, C., D'Agostino, I., Deodato, D., Loregian, A., Grossi, G. et Schenone, S. "3-Cyano-4,6-diphenyl-pyridine amino acid derivatives active as influenza A polymerase inhibitors". IX Giornate Italo-Francesi di Chimica, Genova, 16-18/04/2018.
2. Greco C., Musumeci F., **Giacchello I.**, Perrotti N., Alcaro S., Ortuso F. et Schenone S. "Synthesis of a small library of potential SGK1 inhibitors". IX Giornate Italo-Francesi di Chimica, Genova, 16-18/04/2018.
3. Musumeci, F., Greco, C., **Giacchello, I.**, Crespan, E., Maga, G., Schenone, S., Fallacara, A. L., Molinari, A. et Botta, M. "Pyrazolo[3,4-d]pyrimidines as tyrosine kinase inhibitors: synthesis and biological evaluation". IX Giornate Italo-Francesi di Chimica, Genova, 16-18/04/2018.
4. Greco, 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]pyrimidine as SGK-1 inhibitors". 17th Hellenic Symposium on Medicinal Chemistry, Aristotele University of Thessaloniki, Greece, 1-3/06/2017.
5. **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 (SA), 10-14/09/2017.

6. 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 (SA), 10-14/09/2017.
7. Musumeci, F., Sanna, M., **Giacchello, I.**, Mazzei, M., Schenone, S., Botta, M. "Synthesis of heterocyclic compounds to be tested as potentiators or correctors of mutant CFTR in cystic fibrosis", VI EDWSy (6th European Workshop in Drug Synthesis), Certosa di Pontignano (Siena), 15-19/05/2016.

Congresses Attended

1. IX Giornate Italo-Francesi di Chimica, Genova, 16-18/04/2018.
2. La Giornata della Chimica Ligure. Le attuali tendenze della ricerca chimica in Liguria, Genova 20/10/2017.
3. XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (SA), 10-14/09/2017.
4. VI EDWSy (6th European Workshop in Drug Synthesis), Certosa di Pontignano (Siena), 15-19/05/2016.

Courseware

Courses attended and passed:

Courses Given by Teachers of the Unige:

1. "INN and IUPAC nomenclature of organic drugs". Prof. Giancarlo Grossi (2 credits).
2. "Instrumental techniques for trace elements determination in pharmaceuticals, food products and environmental samples. Prof. Vincenzo Minganti and Prof.ssa Giuliana Drava (2 credits).
3. "Pharmaceutical Biotechnology" Prof. Mauro Mazzei (3 credits).
4. "Design and synthesis of protein-kinase inhibitors as anticancer agents" Prof.ssa Silvia Schenone (2 credits).
5. "Patent and bibliographic databases searching in medicinal chemistry" Prof.ssa Chiara Brullo e Prof.ssa Paola Fossa (2 credits).

Courses Given by invited experts:

1. "Recent advances in computer-aided drug design". Prof. Tuccinardi Tiziano, Univeristà di Pisa, Italia. 16/10/2017.
2. "Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials" and "Novel Materials for energy storage and conversion" Prof. Dr. Thomas Fässler, Department of Chemistry Technical University of Munich, Germany. 11/05/2017.
3. "Functional chromophores-synthesis and applications", Prof. Dr. Thomas J. J. Müller, Heinrich Heine Universität, Düsseldorf. 09-10/06/2016.
4. "Medicinal chemistry with carbohydrates: the influenza virus and the discovery of sialidase inhibitors", Prof.ssa Anna Bernardi, Università degli Studi di Milano. 13/11/2015.

Seminars attended:

1. "Oral diseases and their treatment: an overview". Dott. Kartik Neduri, Università degli Studi di Genova. 15/10/2018.

2. "Five isoforms of N,N,N-tris(tert-butoxycarbonyl)-L-arginine depending on procedure and the investigation of their reactivity in esterification reactions". Dott. Gaby Brice Taptue, Università degli Studi di Genova. 15/10/2018.
3. "Deubiquitinase inhibition as therapeutic strategy". Dott.ssa Vittoria Zoppi, Università degli Studi di Genova. 15/10/2018
4. "The vaccines: from the origins to the present day". Dott.ssa Monica Sanna, Università degli Studi di Genova. 18/10/2017.
5. "Chronic obstructive pulmonary disease (COPD): a pathology overview and the possible effects of particulate matter (PM)". Dott. Daniele Brignole, Università degli Studi di Genova. 18/10/2017.
6. "Imaging in oncology". Dott.ssa Sara Pastorino, Università degli Studi di Genova. 18/10/2017.
7. "Depression: new therapeutic strategy". Dott. Mohamed Sadeghi, Università degli Studi di Genova. 18/10/2017.
8. "Probiotic: properties, uses and interaction with human gut microbiome". Dott.ssa Federica Turrini, Università degli Studi di Genova. 18/10/2017.
9. "New trends in Computer Aided Drug Design" Prof. Tiziano Tuccinardi, Università degli Studi di Pisa. 18/10/2016.
10. "Il marketing cosmetico: dalla mission aziendale alla risposta del consumatore" Dott.ssa Silvia Rum, Università degli Studi di Genova. 18/11/2016.
11. "Odori, profumi e feromoni come mediatori chimici olfattivi" Dott.ssa Chiara Lacapra, Università degli Studi di Genova. 18/11/2016.
12. "Giocare sporco: PAINS e composti promiscui" Dott.ssa Anita Parricchi, Università degli Studi di Genova. 18/11/2016.
13. "Tubercolosi ed altre patologie polmonari: stato dell'arte e recenti sviluppi terapeutici" Dott.ssa Elda Meta, Università degli Studi di Genova. 18/11/2016.
14. "Un caso di proficua collaborazione: biocatalisi e prodotti naturali" Dr. Riva Sergio, Istituto di Chimica del Riconoscimento Molecolare, CNR – Milano. 12/06/2017.
15. "The Biotin-(Strept)avidin system in pretargeting and in biotechnological applications", Dott.ssa Irene Croce, Università degli Studi di Genova. 27/11/2015.
16. "Advanced technologies for the development of physiologically relevant in vitro alternative models", Dott.ssa Jenia Danailova, Università degli Studi di Genova. 27/11/2015.
17. "Palladium-catalyzed reactions: a revolutionary impact in Medicinal Chemistry", Dott. Andrea Desogus, Università degli Studi di Genova. 27/11/2015.
18. "Revolution in the treatment of parasitic diseases: Artemisinin as great scientific goal", Dott.ssa Cinzia M. Francini, Università degli Studi di Genova. 27/11/2015.
19. "Druglikeness and related scoring methods: Ligand Efficiency and Lipophilic Ligand Efficiency", Dott.ssa Sara Guariento, Università degli Studi di Genova. 27/11/2015.
20. "Chemometrics in proteomics studies", Prof.ssa Beata Walczak, Institute of Chemistry, Silesian University, Katowice, Poland. 22/01/2016. "I nutraceutici: I farmaci per le persone sane", Prof. Ettore Novellino, Università degli Studi di Napoli. 26/01/2016.
- 1) "Design of magnetic nanoarchitecture", Prof. Davide Peddis, ISM-CNR - Rome. 22/04/2016.

National and International Schools or Workshops

1. CADD (Computer-Aided Drug Design) Summer School. Università di Pisa, 11-16/07/2016.
2. 5th Workshop "Programma PhD" : "La formazione post lauream e il mondo del lavoro: nell'industria chimica, chi fa ricerca... fa carriera?" Federchimica/Università degli Studi di Genova. Università degli Studi di Genova, Scuola Politecnica. 24/05/2017.
3. European School of Medicinal Chemistry (ESMEC), Urbino, 2-6/07/2017.

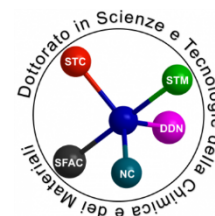
4. Prima giornata di studio: sostenibilità e processi chimici microonde mediate. Gruppo Interdivisionale di Green Chemistry-Chimica sostenibile. 19/10/2018.

Other activities

1. Seminary lesson: "Chemistry in the kitchen: from traditional to molecular cooking". Dipartimento di Farmacia, Università di Genova. 15/10/2018.
2. Tutor of "Physical Chemistry" for the second year course in CTF. September 2017-July 2018.
3. Laboratory assistant for Prof. Elena Cichero in her course "Analysis of drugs I" for second-year students of the Medicinal Chemistry. October-December 2016 and October-December 2017.
4. Laboratory assistant for Michele Tonelli in his course "Analysis of drugs I", for second-year students of the Medicinal Chemistry. October-December 2016.
5. Period of practice in the laboratory at Dipartimento Farmaco Chimico Tecnologico, Università degli Studi di Siena. 07-18/03/2016.
6. Tutor of "Biochemistry" for the second year course in Pharmacy and CTF. September 2016-July 2018.



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



Curriculum: Nanochemistry

EMANUELE LAGO

Start of the Doctorate Program: *November 1st, 2015*

End of the Doctorate Program: *October 31st, 2018*

Advisors: Prof. O. Cavalleri (Unige), Dr. F. Bonaccorso (IIT), Prof. V. Pellegrini (IIT)

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

Thesis abstract

This research theme is devoted to the development of graphene and two dimensional (2D) crystals-based composite materials for flexible electronic, energy conversion and storage, and photonic applications. One of the main targets will be the production of graphene and other 2D crystal inks with controlled morphological and rheological properties. We will develop a top-down synthesis approach for the realization of such inks, which will be first of all studied in detail for what concerns their optical, structural, electrochemical and electrical transport properties. Significant effort will be put in the design of novel composite materials based on graphene and two-dimensional crystal inks and a class of techno-polymers produced both by extrusion process and direct mixing. The graphene and 2D crystals-based polymer composites will be fully characterized by assessing their thermal, optical, structural, electrochemical and electrical transport properties.

ACTIVITY REPORT

Research Activity

The research activity was mainly carried out at the Italian Institute of Technology, Genova

Scientific Publications

Original publications on ISI Journals:

1. **E. Lago**, P. S. Toth, G. Pugliese, V. Pellegrini, and F. Bonaccorso, "Solution blending preparation of polycarbonate/graphene composite: boosting the mechanical and electrical properties", RSC Advances, 6 (2016) 97931

2. A. E. Del Rio Castillo, V. Pellegrini, H. Sun, J. Buha, D. A. Dinh, **E. Lago**, A. Ansaldo, A. Capasso, L. Manna, F. Bonaccorso, "Exfoliation of few-layer black phosphorus in low-boiling-point solvents and its application in Li-ion batteries", *Chemistry of Materials*, 30 (2018) 506
3. E. Petroni, **E. Lago**, S. Bellani, D. W. Boukhalov, A. Politano, B. Gürbulak, S. Duman, M. Prato, S. Gentiluomo, R. Oropesa-Nuñez, J.-K. Panda, P. S. Toth, A. E. Del Rio Castillo, V. Pellegrini, F. Bonaccorso, "Liquid-Phase Exfoliated Indium–Selenide Flakes and Their Application in Hydrogen Evolution Reaction", *Small* 14 (2018) 1800749
4. A. E. Del Rio Castillo, V. Pellegrini, A. Ansaldo, F. Ricciardella, H. Sun, L. Marasco, J. Buha, Z. Dang, L. Gagliani, **E. Lago**, N. Curreli, S. Gentiluomo, F. Palazon, M. Prato, R. Oropesa-Nuñez, P. S. Toth, E. Mantero, M. Crugliano, A. Gamucci, A. Tomadin, M. Polini and F. Bonaccorso, "High-yield production of 2D crystals by wet-jet milling", *Materials Horizons* 5 (2018) 890
5. **E. Lago**, Peter S. Toth, S. Gentiluomo, S. B. Thorat, V. Pellegrini, and F. Bonaccorso, "Enhanced polycarbonate mechanical performances by the addition of few-layers boron nitride with tuneable morphology", submitted
6. **E. Lago**, F. Bonaccorso, S. Gentiluomo, A. E. Del Rio Castillo, N. M. Pugno, R. Cingolani, P. S. Toth, and V. Pellegrini, "Exploiting the ideal properties of two-dimensional fillers for the mechanical reinforcement of polymer nanocomposites", submitted
7. **E. Lago**, A. E. Del Rio Castillo, P. S. Toth, S. B. Thorat, R. Oropesa-Nuñez, S. Colonna, A. Fina, V. Pellegrini and F. Bonaccorso, "On-demand tuning of physical properties of poly(lactic acid) through the addition of 2D crystals", submitted

Communications at Conferences

Oral communications:

1. **E. Lago**, P.S. Toth, V. Pellegrini, and F. Bonaccorso, "Effects of 2D crystals addition on the physical properties of polycarbonate-based composite", presented at GrapheneCanada2016 conference, Montreal (Canada) October 18-20, 2016

Poster Communications:

1. **E. Lago**, P. S. Toth, G. Pugliese, V. Pellegrini, and F. Bonaccorso, "Solution blending preparation of polycarbonate/graphene composite: boosting the mechanical and electrical properties", presented at Graphene2016 conference, Genoa (Italy) April 19-22 2016
2. **E. Lago**, P.S. Toth, S. Gentiluomo, S.B. Thorat, V. Pellegrini, and F. Bonaccorso, "Enhancing polycarbonate performances by adding environmentally friendly liquid-phase exfoliated boron nitride flakes", presented at materials.it conference, Aci-Castello (Italy), December 12-16 2016
3. **E. Lago**, P.S. Toth, S. Gentiluomo, S.B. Thorat, V. Pellegrini and F. Bonaccorso, "Unravelling the boron nitride flakes morphology to enhance polycarbonate performances" presented at Graphene2017 conference, Barcelona (Spain) March 28-31, 2017

Congresses Attended

1. Graphene2016, Genoa (Italy), April 19-22 2016
2. GrapheneCanada2016, Montreal (Canada), October 18-20 2016
3. Materials.it, Catania (Italy), December 12-16 2016
4. Graphene2017, Barcelona (Spain), March 28-April 1 2017

Summer School Attended

1. 8th EPF summer school: "Transport Phenomena in Polymers and Hybrid Materials", Gargnano (Italy), May 14-19 2017

Courseware

Courses attended and passed

1. Basics in Electrochemistry (1 credit)
Speakers: Simone Monaco, Haiyan Sun, Sebastiano Bellani
2. From Crystallography to Imaging (1 credit)
3. Basics of Crystallography and Diffraction by crystals (1 credit)
4. Introductory course on transmission electron microscopy (1 credit)
Speakers: Rosaria Brescia, Zhiya Dang, Joka Buha, Roberto Marotta
5. Opto-Electronic Properties of Semiconductor Quantum Dots (1 credit)
Speaker: Iwan Moreels
6. Science and Technology of 2D Crystals (1 credit)
Speaker: Francesco Bonaccorso
7. Magnetic properties and characterization techniques (1 credit)
Speaker: Aidin La
8. Spectroscopies for chemical analysis (1 credit)
Speakers: Francisco Palazon, Roman Krahne, Sandeep Ghosh
9. Application of Nanocrystals in energy storage, photo-catalysis and heterogeneous catalysis (1 credit)
Speakers: Massimo Colombo, Dipak Shinde, Simone Monaco
10. Nanomaterials synthesis and transformations (1 credit)
Speaker: Luca De Trizio
11. Mechanical properties and atomic force microscopy (1 credit)
Speakers: Luca Ceseracciu and Marco Salerno
12. Electronic properties of solids (3 credits) Speaker: Liberato Manna

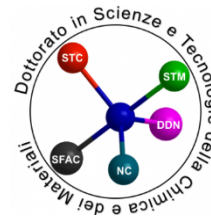
Seminars Attended

1. From sticky tape to industrial products: the challenges of graphene commercialization, Stefano Borini; 11/04/2016
2. Spatio-temporal visualization of atomic motions in low-dimensional materials, Giovanni Maria Vanacore; 03/05/2016
3. First-principle predictions of substrate effect on silicone, Udo Scwingenschloegl; 09/05/2016
4. Graphene and light: from fluorescent molecules to photo-active nanocomposites, Gloria Giudetti; 27/05/2016
5. Nano-photonics phenomena in van der Waals heterostructures, Dmitri N. Basov; 08/06/2016
6. Ionic bonding and the effect of electron repulsion on the band structure, Liberato Manna; 08/06/2016
7. Hybrid nanoscale architectures of semiconductors and carbon nanomaterials, Csaba Janaky; 10/06/2016
8. Combined Light Harvesting and Charge Transfer in Complex Macromolecular Architectures, Amy M. Scott; 14/06/2016
9. Lithium ion batteries: introduction of basic electrochemical cell and lithium ion batteries, Duc Anh Dinh & Lin Chen; 23/06/2016

10. Lithium ion batteries: working mechanism and principle configurations, Duc Anh Dinh & Lin Chen; 22/07/2016
11. Lithium ion batteries: electrodes of lithium batteries, Duc Anh Dinh & Lin Chen; 29/07/2016
12. Halocarbons in Nanomedicine and Nanotechnology: New Opportunities and Challenges, Pierangelo Metrangolo; 07/10/2016
13. From chemical complexity to functional complexity: tailoring multifunctional low dimensional materials and devices, Paolo Samorì; 14/11/2016
14. Visualizing and controlling optoelectronic processes in lead halide perovskites, Alexander Weber; 14/11/2016
15. van der Waals Assembly of 2D Materials for Device Applications, Gwan-Hyoung Lee; 16/01/2017
16. Mesoscopic thermodynamics, Klaus Ensslin; 07/02/2017
17. Structural biopolymers – using nature’s building blocks as an inspiration for advanced manufacturing, Benedetto Marelli; 01/03/2017
18. Graphene-based membranes, Slaven Garaj; 11/04/2017
19. Integrated Photoelectrodes for CO₂ reduction and water oxidation, Francesca Maria Toma; 12/06/2017
20. The Electrochemical & Physical Performance Benefits of Graphene into Li-ion Energy Storage Technologies, Melanie Loveridge; 15/09/2017
21. The Graphene and other 2D related materials interface engineering for highly efficient and stable organic and perovskite solar cells, Emmanuel Kymakis; 14/11/2017
22. Membrane engineering, Enrico Drioli; 05/02/2018



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



Curriculum: Materials Science and Technology

MICHELE MAGNOZZI

Start of the Doctorate Program *November 1st, 2015*
End of the Doctorate Program *October 31st, 2018*
Advisors: Prof. Maurizio Canepa, Dr. Francesco Bisio
Thesis Title: Optical properties of composite plasmonic nanomaterials

Thesis abstract

In recent years, the rise of thermoplasmonics has sparked a new interest towards the temperature-dependent optical properties of systems based on noble metals. However, the majority of data available in the literature have been collected decades ago on bulk systems, which behave quite differently from the respective nano-sized counterparts. In this thesis we present a thorough investigation of the temperature-dependent optical properties of ordered arrays of noble-metal nanoparticles, studied with a very sensitive optical technique (spectroscopic ellipsometry) in their most favorable environment (high vacuum or liquid). We apply dedicated models to identify, describe and explain the variations induced by the temperature, and, as a consequence of proper modelling, we are able to provide a complete description of the complex, anisotropic optical properties of our nanoparticles lattices in a wide range of temperatures

ACTIVITY REPORT

Research Activity

Scientific Publications

1. **M. Magnozzi**, M. Ferrera, M. Canepa, F. Bisio. Monitoring the solid-state dewetting of densely packed arrays of Au nanoparticles. Accepted by Journal of Physics: Conference Series, 2018.
2. P. Parisse, I. Solano, **M. Magnozzi**, F. Bisio, L. Casalis, O. Cavalleri, M. Canepa. Thickness and beyond. Exploiting spectroscopic ellipsometry for the investigation of ultrathin interfaces of biological interest. Chapter in book: Ellipsometry of functional organic surfaces and films, K. Hinrichs and K.-J. Eichhorn (editors), Springer 2018.
3. M. Agostini et al., The Monte Carlo simulation of the Borexino detector. *Astropart. Physics*, 97, 136-159, 2018.

4. **M. Magnozzi**, S. Terreni, L. Anghinolfi, M. Neri, I. Solano, M.M. Carnasciali, S. Uttiya, G. Gemme, M. Canepa. Optical properties of amorphous SiO₂-TiO₂ multi-nanolayered films for 1064 nm mirror technology. *Optical materials*, 75, 94-101, 2018.
5. S. Forti, A. Rossi, H. Buch, T. Cavallucci, F. Bisio, A. Sala, T. Montes, A. Locatelli, **M. Magnozzi**, M. Canepa, K. Mueller, S. Link, U. Starke, V. Tozzini, C. Coletti. Electronic properties of single-layer tungsten disulfide on epitaxial graphene on silicon carbide. *Nanoscale*, 9, 16412-16419, 2017.
6. F. Bisio, E. Principi, **M. Magnozzi**, A. Simoncig, E. Giangrisostomi, R. Mincigrucci, L. Pasquali, C. Masciovecchio, F. Boscherini, M. Canepa. Long-lived nonthermal electron distribution in aluminum excited by femtosecond extreme ultraviolet radiation. *Physical Review B*, 96, 081119(R), 2017.
7. **M. Magnozzi**, N. Haghighian, V. Miseikis, C. Coletti, F. Bisio, M. Canepa. Fast detection of water nanopockets underneath wet-transferred graphene. *Carbon*, 118, 208-214, 2017.
8. **M. Magnozzi**, F. Bisio, M. Canepa. Solid-state dewetting of thin Au films studied with in situ spectroscopic ellipsometry. *Applied Surface Science*, 421, 651-655, 2017.
9. **M. Magnozzi**, M. Ferrera, L. Mattera, M. Canepa, F. Bisio. Plasmonics of Au nanoparticles in hot thermodynamic bath. Submitted to *Nanoscale* Under review:

Communications at Conferences

Oral Communications

1. 65th AVS Symposium, 22.10.2018, Long Beach, USA. **Spectroscopic ellipsometry investigation of temperature effects in heated self-organized 2D arrays of Au nanoparticles.**
2. 9th Young Researcher Meeting, 11.07.2018, Salerno. **Spectroscopic ellipsometry investigation of temperature effects in heated self-organized 2D arrays of Au nanoparticles.**
3. 10th Workshop Ellipsometry, Chemnitz, Germania, 19.-21.03.2018. **Fast detection of water nanopockets underneath wet-transferred graphene.**

Poster Communications:

1. M. Magnozzi, M. Ferrera, M. Canepa, F. Bisio. **Temperature-dependent optical properties of plasmonic nanosystems.** Presented at the conference NANOP 2018 in Rome (01-03 October, 2018).
2. M. Magnozzi, M. Ferrera, M. Canepa, F. Bisio. **Plasmonic properties of heated self-organized 2D arrays of Au nanoparticles.** Presented at the Plasmonica Workshop in Firenze (04-06 July, 2018).
3. M. Ferrera, M. Magnozzi, F. Bisio, M. Canepa. **Temperature-dependent optical constants of noble metals Au and Ag.** Presented at the Plasmonica Workshop in Firenze (04-06 July, 2018).
4. M. Magnozzi, Y. Brasse, T. Koenig, F. Bisio, A. Fery, M. Canepa. **Plasmonic properties of self-assembled Au/PNIPAM core-shell nanoparticles studied with spectroscopic ellipsometry.** Presented at the Plasmonica Workshop in Firenze (04-06 July, 2018).
5. M. Magnozzi, Y. Brasse, T. Koenig, F. Bisio, A. Fery, M. Canepa. **Spectroscopic ellipsometry analysis of self-assembled Au/PNIPAM core-shell nanoparticles.** Presented at the 10th Workshop Ellipsometry in Chemnitz (19-21 March, 2018)
6. M. Magnozzi, M. Ferrera, M. Canepa, F. Bisio. **Temperature-dependent optical properties of plasmonic nanosystems.** Presented at the 10th Workshop Ellipsometry in Chemnitz (19-21 March, 2018).
7. M. Magnozzi, S. Terreni, L. Anghinolfi, S. Uttiya, M.M. Carnasciali, G. Gemme, M. Neri, M. Principe, I. Pinto, L.-C. Kuo, S. Chao, M. Canepa. **Optical properties of amorphous SiO₂-TiO₂ multi-nanolayered films for 1064 nm mirror technology.** Presented at the 10th Workshop Ellipsometry in Chemnitz (19- 21 March, 2018).

8. M. Magnozzi, D. Catone, P. O'Keefe, A. Paladini, F. Toschi, A. Alabastri, R. Proietti Zaccaria, M. Canepa, F. Bisio. **Ultrafast laser-induced nanoparticle melting**. Presented at the workshop "Plasmonica 2017" in Lecce (5-7 July, 2017).
9. M. Magnozzi, F. Bisio, M. Canepa. **Temperature-dependent plasmonic properties of self-assembled Au NPs arrays**. Presented at the workshop "Plasmonica 2017" in Lecce (5-7 July, 2017).
10. M. Magnozzi, F. Bisio, M. Canepa. **High vacuum, mini chamber for real time, in situ Spectroscopic Ellipsometry**. Presented at the conference "ICSE-7" in Berlin (6-10 June, 2016).
11. A. Amato, M. Magnozzi, M. Neri, S. Terreni, G. Gemme, M. Canepa. **Spectroscopic Ellipsometry characterization of high-quality oxide coatings for gravitational wave detectors**. Presented at the conference "GWADW 2016" in Isola d'Elba (22-28 May, 2016).
12. M. Magnozzi, V. Miseikis, C. Coletti, F. Bisio, M. Canepa. **Thermal annealing of chemical vapour deposited graphene studied with spectroscopic ellipsometry**. Presented at the conference "Graphene 2016" in Genova (19-22 April, 2016).
13. F. Bisio, E. Principi, M. Magnozzi, A. Simoncig, E. Giangrisostomi, R. Mincigrucchi, L. Pasquali, F. Boscherini, C. Masciovecchio, M. Canepa. **All-optical pump-probe study of ultrafast dynamics in FEL-excited aluminum**. Presented at the conference "Science@FELs 2016" in Trieste (5-7 September, 2016).

Congresses Attended

1. 65th AVS Symposium, Long Beach (USA) 21-27 October, 2018
2. NANOP 2018, Rome 1-3 October, 2018
3. International Conference of Spectroscopic Ellipsometry (ICSE-7), Berlin (Germany) 6-10 June, 2016
4. Science@FELs 2016, Trieste 5-7 September, 2016
5. Graphene 2016, Genova 19-22 May, 2016

Courseware

Courses attended and passed

1. "Fondamenti di microscopia elettronica a scansione ed in trasmissione". Prof. Riani. (3 credits)
2. "Materiali Organici per l'Elettronica, l'Optoelettronica e la Fotonica". Prof. Comoretto (2 credits)
3. "Caratterizzazione di nanoparticelle per mezzo della microscopia a forza atomica e Dynamic Light Scattering". Prof. Rolandi (2 credits)
4. "Introduction to the applications of Raman Spectroscopy to Materials". Prof.ssa Carnasciali (2 credits)
5. "Elements of Soft Matter". Prof.ssa Relini (2 credits)

National and International Schools or Workshops

1. "3rd NIC@IIT Practical Workshop on Advanced Microscopy" (IIT, Genova, 12-16 December 2016)
2. "Winter school – New Frontiers in 2D Materials" (Villard-de-Lans, France, 15-20 January 2017)
3. "10th Workshop Ellipsometry", Chemnitz (Germany), 19-21 March 2018)
4. "Plasmonica 2018" (Firenze, 4-6 July 2018)
5. "Plasmonica 2017" (Lecce, 5-7 July 2017)
6. "Plasmonica 2016" (Genova, 14-16 September 2016)

Seminars Given

1. Spectroscopic ellipsometry: a tool to investigate self-assembled optical metasurfaces. Seminario presso il Leibniz Institut fur Polymerforschung, Dresda, Germany, 21.06.2018.

2. DAAD Stipendiatentreffen, Dresda, Germany, 30.11.2017. Nanothermometer without display – a metasurface approach.
3. Optical properties of Graphene and Graphene-like materials. Seminario da me tenuto all'interno del corso "Metodi ottici spettroscopici per lo studio dei materiali", Prof. Maurizio Canepa. 23.05.2017
4. Proprietà ottiche del Grafene. Seminario da me tenuto all'interno del corso "Metodi ottici spettroscopici per lo studio dei materiali", Prof. Maurizio Canepa. 23.05.2016

Seminars Attended

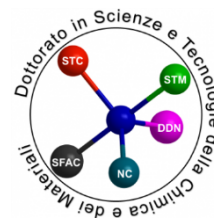
1. "Quantum thermodynamics in strongly coupled quantum dots" Dr. Thomas Schmidt, DIFI, 10.09.2018
2. "Stimulus triggered reconfigural microstructures from responsive polymer" Dr. Yu Ye, IPF Dresdem, 22.05.2018
3. "Engineering of surfaces and thin layer systems by laser, electron and ion beam" Dr. Pierre Lorenz, IPF Dresden, 17.05.2018
4. "Biomimetic complex systems for soft actuation and neural computing" Prof. Milani, DIFI, 10.05.2018
5. "Plasmon-enhanced hot carrier generation and extraction" Charlene Ng, IPF Dresden, 07.05.2018
6. "From proteins at interfaces to silica, passing through membranes" Grazia Gonella, DIFI, 16.03.2018
7. "Designer structure and morphology at the 2D level: from Xenex to anisotropic MoS₂ nanosheets" Dr. Alessandro Molle, DIFI, 08.03.2018
8. "Non-reciprocal light propagation in macroscopic self-assembled gain-loss nanomaterials" Vaibhav Gupta, IPF Dresden, 02.11.2017
9. "Plasmon excitations in quasi-one dimensional atomic wires". Prof. Herbert. Pfner, DIFI, 19.07.2017
10. "How to write great papers and get published". S. Munau, DIFI, 12.07.2017
11. "First results from the current observation run of the LIGO-Virgo network of advanced gravitational waves detectors. Fiodor Sorrentino, DIFI, 20.06.2017.
12. "Analisi termica accoppiata alla gas cromatografia e spettrometria di massa". Federico Locardi, DCCI. 13.06.2017
13. "Structural study of RE-doped ceria and of filled skutterodites: the contribution of micro-Raman spectroscopy". Cristina Artini, DCCI. 01.06.2017
14. "La_{0.7}Sr_{0.3}MnO₃ thin films for sensing applications". Laurence Mechin, Normandie Univ., DIFI, 30.05.2017
15. "Ion Beam Analysis per lo studio dei materiali: sviluppi recenti e applicazioni". A. Zucchiatti, Universidad Autonoma de Madrid. 10.10.2016
16. "Onde gravitazionali: un nuovo sguardo sull'universo". G. Gemme, INFN. 15.02.2016

Other Activities

1. Research activity at Leibniz Institut für Polymerforschung (Dresden, Germany), Sept-Dec 2017 and Apr-June 2018.
2. Research activity at the FERMI Free Electron Laser (Basovizza, Trieste), 30.10-01.11.2016
3. Research activity at the ELETTRA Synchrotron (Basovizza, Trieste), 24-28.05.2016
4. Teaching support (20 hrs) for the General Physics II course at the Naval Engineering school (Prof. Edvige Celasco), 01.03-31.05.2016
5. Lab support for the high school students' stages, 02.2018
6. Supervision of the experimental activity of a student working towards bachelor's degree (Andrea Mandich, Materials Science)



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



Curriculum: Pharmaceutical, Food and Cosmetic Sciences

KHARTIK NEDURI

Start of the Doctorate Program *November 1st, 2015*
End of the Doctorate Program *October 31st, 2018*
Advisor: Prof. Gabriele Caviglioli
Thesis Title: Development and evaluation of novel buccal dosage forms

Thesis abstract

The buccal region of the oral cavity is an attractive and easily accessible site for therapeutic agents for local and systemic delivery due to the several advantages like avoidance of the first pass metabolism, localization of dosage form in the site of administration and allowing direct absorption through the mucosa.

The buccal dosage forms can be useful in different therapies and in patients of different ages.

In children therapies, a buccoadhesive fast dissolving film containing mini-pellets could be a way to overcome swallowing problems related to the size of dosage form. Additionally, in pediatric field, buccal formulations represent an attractive alternative for non-invasive delivery of potent but labile biotechnological drug, such as those used in vaccination.

Moreover, less cooperative elderly patients could be treated by a sweet fast dissolving buccal dosage forms. Buccoadhesive dosage forms can be used for systemic delivery of analgesics for the treatment of pain relief, improving drug bioavailability by mucosal absorption or for local delivery both in dental diseases, like gingivitis, periodontitis, and in mucosal injury from chemotherapy and radiotherapy.

The dosage forms will be prepared by compression or partly encapsulating pelletized solid dosage forms, like granules, nonpareils, mini-tablets (coated, uncoated, single or multiple units) in buccal films, also investigating aspects related to safety, palatability and patient compliance. These dosage forms can be prepared by solvent-casting method. For the fabrication of films, plasticizers (propylene glycol, glycerin, polyethylene glycols) sweeteners (sucralose, aspartame, mannitol), flavoring agents (menthol, vanillin, clove oil, orange) polymers for adhesive layer (HEC, HPC, polyvinylpyrrolidone, polyvinylalcohol, carbopol), diluents (lactose DC, microcrystalline starch, starch), permeation enhancers (surfactants, bile salts, fatty acids) and various polyhydric alcohols such as sorbitol and xylitol can be used. Mini-pellets can be prepared by various methods like

spray drying, dry granulation or direct compression and coated where necessary. Then they are said to be encapsulated in films and tablets.

The prepared dosage forms will be characterized and subjected to *in-vitro* evaluation tests.

ACTIVITY REPORT

Research Activity

The research activity was mainly carried out at the Department of Pharmacy (DIFAR)

Scientific Publications

Original publications on ISI Journals:

1. Development and characterization of a mucoadhesive sublingual formulation for pain control: extemporaneous oxycodone films in personalized therapy. *Drug Development and Industrial Pharmacy* (2017).

Communications at Conferences

Oral communications:

1. "Formulation development of a biopolymer-based multilayer film for the local treatment and wound repair of periodontitis", Innovation in local drug delivery school, 25-28 September 2018, Como, Italy.

Poster Communications:

1. "Norbiotinamine as coupling agent for pretargeting: improvement of preparative reaction (optimization)", 4-7 April 2016, 10th world meeting on pharmaceuticals, biopharmaceutics & pharmaceutical technology, Glasgow, UK.
2. "Buccoadhesive polymeric films for oromucosal oxycodone delivery in acute pain control", 5-8 September 2016, University of Calabria, Arcavacata di Rende (CS).
3. Optimization of a parenteral thermoresponsive formulation based on metformin hydrochloride. 3-4 April 2017, 2nd European conference on pharmaceuticals, Krakow, Poland.
4. Preformulation study of multilayer films for local treatment of oral diseases, 25-28 September 2017, Advanced school in nanomedicine, Pula, Italy.
5. Characterization of macroporous hydrogel scaffolds for 3D cell culture in preclinical studies, 11th World Meeting on Pharmaceuticals, Biopharmaceutics and Pharmaceutical Technology, March 19-22, Granada, Spain, 2018.
6. Multilayer films for treatment of oral diseases: a preliminary study, CRS Annual meeting & Exposition, July 22-24, New York city, USA 2018.
7. A study on liposomal formulation. Innovation in local drug delivery school, 25-28 September 2018, Como, Italy.

Congresses Attended

1. 2nd European conference on pharmaceuticals, Krakow, Poland, 3-4 April 2017.
2. 11th World Meeting on Pharmaceuticals, Biopharmaceutics and Pharmaceutical Technology, March 19-22, Granada, Spain, 2018.

3. Medicines for older people: Advances in drug delivery, 12th A.It.U.N meeting, Bologna, 10-11 may 2018.
4. CRS Annual meeting & Exposition, July 22-24, Newyork city, USA 2018

Courseware

Type B courses

1. Metodi di preparazione e controllo di forme farmaceutiche innovative (Docenti: G.Caviglioli, S.Baldassarri, B.Parodi, E.Russo): 2 CFU
2. Metodologia della ricerca sperimentale (Docenti:M.Grotti, R.Leardi) : 3 CFU
3. Tecniche strumentali per la determinazione di elementi in traccia di interesse farmaceutico, alimentare, ambientale (Docenti: V.Minganti, G.Drava) : 2 CFU
4. Marker molecolari della qualità e della genuinità degli alimenti(Docenti: R.Boggia, P.Zunin) : 2 CFU

Type A courses:

1. Superhard materials: structural chemistry of boron and borides(6/08/17 & 7/08/17)(Rogl, Universita' di Vienna, Austria) :1CFU
2. Global vision of biotechnology (26/06/17)(Josa Manuel Domanguez Gonzalez, Universita' di Vigo, Spagna) :1CFU
3. Publishing papers and strategies to visualize the scientific productivity(27/06/17) Josa Manuel Domanguez Gonzalez, Universita' di Vigo, Spagna) :1CFU
4. Chemometrics in proteomics (Beata Walczak)(DIFAR 22/1/2016)

National and International Schools or Workshops:

1. Advanced school in nanomedicine, 25-28 September 2017, pula, Italy.
2. Intensive patent workshop: How to draft, analyze and circumvent a formulation patent, APV GmbH, Berlin, Germany, February 2018.
3. Innovation in local drug delivery school, 25-28 September 2018, Como, Italy.

Seminars Attended :

1. "The Biotin-(Strept)avidin system in pretargeting and in biotechnological applications", Irene Croce, (DIFAR 27/11/2015).
2. "Advanced technologies for the development of physiologically relevant in vitro alternative models", Jenia Dainalova, (DIFAR 27/11/2015).
3. "Palladium-catalyzed reactions: a revolutionary impact in Medicinal Chemistry", Andrea Desogus, (DIFAR 27/11/2015).
4. "Revolution in the treatment of parasitic diseases: Artemisinin as great scientific goal", Cinzia M. Francini, (DIFAR 27/11/2015).
5. "Druglikeness and related scoring methods: Ligand Efficency and Lipophilic Ligand Efficency", Sara Guariento, (DIFAR 27/11/2015)
6. "Il marketing cosmetico: dalla mission aziendale alla risposta del consumatore",Dr.ssa Silvia Rum (DIFAR 18/11/2016)
7. "Odori, profumi e feromoni come mediatori chimici olfattivi",Chiara Lacapra (DIFAR 18/11/2016).
8. "Giocare sporco: PAINS e composti promiscui"Anita Parricchi, (DIFAR 18/11/2016).
9. "Tubercolosi ed altre patologie polmonari: stato dell'arte e recenti sviluppi terapeutici", Elda Meta, (DIFAR 18/11/2016).

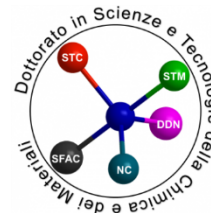
10. "The vaccines: from the origins to the present day" Sanna Monica (DIFAR 18/10/2017).
11. "Chronic Obstructive Pulmonary Disease (COPD): a pathology overview and the possible effects of Particulate Matter (PM)". Brignole Daniele (DIFAR 18/10/2017).
12. "Imaging in Oncology". Pastorino Sara (DIFAR 18/10/2017).
13. "Depression: new therapeutic strategies", Sadeghi Mohamed, (DIFAR 18/10/2017).
14. "Probiotics: properties, uses and interaction with human gut microbiome". Turrini Federica, (DIFAR 18/10/2017)
15. "Stimolazione elettrica "dinamica" del midollo spinale: una nuova strategia per modulare i circuiti locomotori spinali" .Dott. Giuliano Taccola, (DIFAR 21/12/18).
16. "Chemistry in the kitchen from traditional to molecular cooking".Dott.Giachello.Illaria,(DIFAR 15/10/18).
17. Five isoforms of N,N,N-tris(tert-butoxycarbonyl)-L-arginine depending on procedure and the investigation of their reactivity in esterification reactions" Dott. Gaby Brice Taptue, (DIFAR 15/10/18).
18. "Deubiquitinase inhibition as therapeutic strategy"Dott.ssa Vittoria Zoppi, (DIFAR 15/10/18).

Other Activities

1. Elsevier event: How to write a successful scientific paper (17/07/16).
2. Certification course in Drug Development, University of California, San Diego, USA (19/11/2016).
3. General Course on Intellectual Property. World intellectual property organization (WIPO), Geneva, Switzerland (17/11/2016).
4. Laboratory assistant –Pharmaceutical technology & Legislation (2016-2017)
5. Laboratory assistant –Pharmaceutical technology & Legislation (2017-2018)



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



Curriculum: Nanochemistry

MILAN PALEI

Start of the Doctorate Program *1st November, 2015*

End of the Doctorate Program..... *31st October, 2018*

Advisors: Dr. Roman Krahné (IIT), Dr. Stefan Kudera (IIT), Prof.
Francesco Buatier de Mongeot, Unige

Thesis Title: Optoelectronic and Plasmonic effects in Nanocrystals

Thesis abstract

Colloidal semiconductor nanocrystals can be excellent light emitters or absorbers where the optical properties as for example the light emission wavelength, direction and polarization can be controlled via the nanocrystal size, shape and composition. This makes them very interesting as active material in light emitting, lasing, or photovoltaic devices. On the other hand, metal nanostructures are very good conductors and are used for electronically contacting other nanomaterials. Additionally they can strongly interact with light in the visible and infrared spectral regions. The unique properties of these plasmon oscillations of their free electrons gave rise to the field of nanoplasmonics. Therefore the use of metals in hybrid structures can go well beyond their use as electric leads or interconnects.

This project aims at combining the favorable properties of both worlds in order to investigate complex optoelectronic systems and to pave the way for novel architectures for components in photodetectors, optical communication, photovoltaics, and nanoscale electronics.

ACTIVITY REPORT

Research Activity

The research activity was mainly carried out at the Italian Institute of Technology, Genova

Scientific Publications

Original publications on ISI Journals:

1. **Palei, Milan**, Vincenzo Caligiuri, Stefan Kudera, and Roman Krahné. "Robust and Bright Photoluminescence from Colloidal Nanocrystal/Al₂O₃ Composite Films fabricated by Atomic Layer Deposition." ACS applied materials & interfaces (2018)

2. Caligiuri, Vincenzo, **Milan Palei**, Muhammad Imran, Liberato Manna, and Roman Krahné. "Planar Double-Epsilon-Near-Zero Cavities for Spontaneous Emission and Purcell Effect Enhancement." ACS Photonics (2018)
3. Shinde, Dipak V., Zhiya Dang, Urko Petralanda, **Milan Palei**, Mengjiao Wang, Mirko Prato, Andrea Cavalli, Luca De Trizio, and Liberato Manna. "In Situ Dynamic Nanostructuring of the Cu–Ti Catalyst-Support System Promotes Hydrogen Evolution under Alkaline Conditions." ACS applied materials & interfaces 10, no. 35 (2018): 29583-29592

Communications at Conferences

Oral communications:

1. Presented at SPIE Nanoscience + Engineering conference paper entitled "**Enhance optoelectronics properties of colloidal quantum dots infilled in Al₂O₃ using atomic layer deposition**" held in San Diego, California from 6-10th August, 2017

Poster Communications:

1. International Conference on Physics of Semiconductor (34th ICPS, Poster), 29th July-3rd Aug 2018, Montpellier, France

Courseware

Courses attended and passed

1. "Electronic properties of solids", Prof. Manna L. (2, 9, 16, 23 March, 1, 13, 20, 27 April and 4, 11, 16 May 2016, IIT) – 3 credits.
2. "Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations", Dr. De Trizio L. (19, 21 April, 2 May 2016, IIT) – 1 credit.
3. "Electric circuits for Electrochemistry", Ansaldo A., Monaco S. (3, 10, 17, 24, 31 May, IIT) – 3 credits.
4. "Basics of Crystallography and Diffraction by crystals", Dr. Prato M. (20, 25, 30 May 2016, IIT) – 1 credit.
5. "Introductory course on transmission electron microscopy", Dr. Brescia R., Dr. Marotta R., Dang Z. (10, 17, 21, 30 June 2016, IIT) – 1 credit.
6. "Magnetic properties and characterization techniques", Dr. Lak A. (13, 20, 23 September 2016, IIT) – 1 credit.
7. "Opto-Electronic Properties of Semiconductor Quantum Dots", Dr. Iwan Moreels (6,13,20,25 July 2016, IIT) – 1 credit
8. "Science and technology of 2D crystals", Dr. Francesco Bonaccorso (4,12,19,26 July 2016, IIT)- 1 credit
9. "Nano-plasmonic devices: from fabrication to applications", Dr. Andrea Toma (13,25,27th October 2016, IIT)-3 credit
10. " Spectroscopies for chemical analysis", Dr. Francisco Palazon, Prof. Roman Krahné, Dr. Sandeep Ghosh (4, 11, 18th October 2016, IIT)- 1 credit
11. "Advanced Optical Fluorescence Microscopy Methods I", Prof. Alberto Diaspro (29, 30, 31st May 2017, IIT)- 3 credit

National and International Schools or Workshops

1. Summer School: School of Photonics 2016: "Plasmonics and Nano-optics" (10-14 July, 2016, Cortona) (yet to be credited by university)

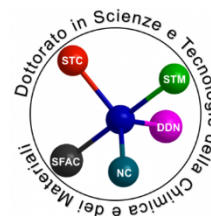
2. Workshop: PLASMONICA 2016:Workshop in Plasmonics (14-16 Sept, 2016, IIT Genova)(yet to be credited by university)
3. Winter School: EUPROMETA-35th Doctoral School in Metamaterials, 18th-22nd December 2017, Roma Tre University, Rome, Italy (yet to be credited by university)
4. Workshop: Workshop on dry processing for Nanoelectronics and Micromechanics: Deposition and etching organized by Oxford Instruments Plasma Technology and RWTH Aachen held from 20 to 21st September, 2017 at RWTH Aachen, Aachen, Germany.(yet to be credited by university)

Seminars Attended

1. Dr. G.M Vanacore, "Spatio-temporal visualization of atomic motion in low-dimensional materials", IIT, 3rd May, 2016
2. Prof. D.N. Basov, " Nano-photonics phenomena in Vanderwaal Heterostructures", IIT, 8th June, 2016
3. Prof. U. Schwingenschögl, " First Principle prediction of Substrate effects on Silicone", IIT, 09th May, 2016
4. Dr. A. G. Kanaras, " Colloidal nanoparticles and applications", IIT, 28th April, 2016
5. Dr. I Bakaimi, " Hydration induced spin glass state in a frustrated Na-Mn-O triangular lattice, IIT, 28th April, 2016
6. Dr. Paolo Samori, " From Chemical complexity to functional complexity: tailoring multifunctional low dimensional materials and devices", IIT, 14th Nov, 2016
7. Alexander Weber-Bargioni, "Visualizing and controlling optoelectronics processes in lead halide perovskites", IIT, 14th November, 2016
8. Dr. Takahiro Ikeda, " Application of nanocrystals to photocatalysis and exhaust gas purification", IIT, 1st February, 2017
9. Prof. Nicola Armaroli, "Photoactive systems for solar energy conversion, luminescence and catalysis",IIT, 27th January, 2017
- 10.Dan Oron, " Colloidal double quantum dots", IIT, 14th February, 2017
- 11.Dmitri Talapin "Synthetic methodology for colloidal nanomaterials: limitations and opportunities,IIT, 26th May, 2017
- 12.Federic Capasso,"Flat Optics Based Metasurface", IIT, 13th December, 2017
- 13.Prof.Craig B. Arnold," Jet formation and Control in laser induced forward transfer printing in liquid inks", IIT, 2nd July, 2018
- 14.Gabriele Grosso,"Quantum Optics with two-dimensional materials: from many body physics to quantum information",IIT, 17th April, 2018
- 15.Dr. Andrea Marini," Nonlinear Nanophotonics with 2d materials and near-zero index media", IIT, 19th July, 2018
- 16.Dr. Stavros Pissadakis,"Lab in Fiber: Photonic Devices", IIT, 21st May, 2018
- 17.Dr.Philip Schaefer, "Scattering-Type scanning Near-field Optical Microscope for various application", IIT, 27th February, 2018
- 18.Francesco Scotognella,"Photophysics and Photonic applications of alternative plasmonic nanomaterials", IIT, 5th April, 2018



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



Curriculum: Nanochemistry

LEA PASQUALE

Start of the Doctorate Program: 1st November, 2015
End of the Doctorate Program: 30th April, 2019
Advisors: Prof. L. Manna (IIT), Dr. M. Colombo (IIT),
Prof. R. Ferrando (UNIGE)
Thesis Title: Bimetallic Nanoparticles as Catalyst for Energy-Related Processes

Thesis abstract

Nanotechnology is rapidly developing and the setup of methods for the synthesis of metallic nanocrystals (NCs) with controlled functional activity is a great challenge. My PhD research project is aimed at the study of bimetallic NCs as catalysts for preferential oxidation (PROX) of CO. The CO PROX is one of the most suitable methods for purification of H₂ streams for example from renewable biomass sources. The removal of CO is important in order to use H₂ in fuel cells as CO is highly poisonous for the Pt anode of the fuel cell. For this reason its content has to be reduced below 10 ppm. The challenge is to prepare a catalyst with high activity at low temperatures (80–200 °C) and high selectivity towards CO oxidation, avoiding the oxidation of H₂. There's already a lot of work done in the literature on this topic. However, for bimetallic NCs some aspects still need to be deeply investigated, such as the role of the support and the gas atmosphere in the phase segregation of bimetallic NCs. Indeed, as an example, a previous study conducted by our group reported the structural changes of AuCu NCs supported on alumina upon different redox treatments and their effects on the CO oxidation reaction. The work highlighted how the catalytic activity strictly depended on the operating atmosphere, which induced structural changes such as phase segregation and Cu species migration on the support surface. As an extension of this work, thus, different supports, phase segregation under different atmospheres and metal migration on the support were studied for other two families of bimetallic NCs. All these phenomena can affect indeed the activity and the selectivity of the catalyst.

For this purpose, PdCu and PtCu bimetallic NCs were synthesized by means of wet chemistry method, in order to control size, shape, and composition. The as-synthesized bimetallic NCs were anchored on different supports such as Al₂O₃ and SiO₂, and then, subjected of a dedicated study where their transformations upon different pre-treatments under oxidizing or reducing atmospheres were deeply investigated. The transformations that the NCs underwent upon different activation treatments were correlated with the catalytic activity. The catalysts were characterized by means of common techniques such as TEM, XRD, SAED and STEM-HAADF-EDS to investigate the composition, structure and morphology of the prepared materials and to study the

transformations and identify the nature of the active sites. Besides ex-situ characterization of the tested catalytic materials, operando and in situ studies were also performed such as in situ DRIFTS Spectroscopy by the probe molecule of CO and in situ X-ray Absorption Spectroscopy with synchrotron radiation source.

The main outcomes of the research work are the development of novel catalytic materials active in the selected reaction, the identification of the structure-activity relationship for the studied bimetallic NCs and the improved understanding of reaction mechanisms of CO PROX

ACTIVITY REPORT

Research Activity

The research activity was mainly carried out at the Italian Institute of Technology (IIT), Genoa Italy

Scientific Publications

1. P. Destro, T. Kokumai, A. Scarpellini, **L. Pasquale**, L. Manna, M. Colombo, D. Zanchet; "The crucial role of the support in the transformations of bimetallic nanoparticles and catalytic performance"; ACS Catal. 2018, 8, 1031-1037.
2. **L. Pasquale**, S. Najafshirtari, R. Brescia, A. Scarpellini, L. Manna, M. Colombo; "Gas atmosphere induced structural changes of bimetallic noble metal-copper nanocrystals: the role of the noble metal" (under preparation).
3. **L. Pasquale**, S. Najafshirtari, R. Brescia, A. Scarpellini, L. Manna, M. Colombo; "Revealing the synergy between oxide and alloy phases on the performance of bimetallic PdCu and PtCu catalysts for CO oxidation reaction" (under preparation).

Communications at Conferences

Oral Communications

1. "Effect of redox treatments on the structure evolution of γ -Al₂O₃ supported bimetallic noble metal copper nanocrystal catalysts" L. Pasquale, R. Brescia, A. Scarpellini, L. Manna, M. Colombo. International Meeting on Nanoalloys IMN 2018, 22nd-25th May 2018, Orléans, France.

Poster Communications

1. "The role of the noble metal in the transformations of supported copper-based bimetallic nanocrystals upon oxidative or reductive pre-treatments." L. Pasquale, L. Manna, M. Colombo. North American Catalysis Society Meeting 2017 (NAM25), 4th-9th June 2017, Denver, Colorado.
2. "Gas atmosphere induced structural changes of bimetallic noble metal-copper nanocrystals: the role of the noble metal." L. Pasquale, R. Brescia, A. Scarpellini, L. Manna, M. Colombo. Catalysis Fundamentals and Practice Summer School 17th-21st July 2017, Liverpool, UK.
3. "The effect of red-ox treatments on the catalytic activity of PtCu and PdCu NCs: an in-situ DRIFTS study." L. Pasquale, L. Manna, M. Colombo. 13th European Congress on Catalysis (EUROPACAT 2017). 27th-31st August, Florence, Italy.
4. "Dynamic structural changes of γ -Al₂O₃ supported bimetallic noble metal-copper nanocrystal catalysts over redox treatments". L. Pasquale, R. Brescia, A. Scarpellini, L. Manna, M. Colombo. Designing Nanoparticle Systems for Catalysis Faraday Discussion, 16th – 18th May 2018, London, United Kingdom.

5. "Probing the evolution of PdCu and PtCu bimetallic nanocrystal catalysts under operando conditions by in-situ X-ray absorption spectroscopy." L. Pasquale, S. Najafshirvani, R. Brescia, A. Scarpellini, L. Manna, M. Colombo. International Meeting on Nanoalloys IMN 2019, 4th-7th June 2019, Genova, Italy.

Courseware

Courses attended and passed

General Courses: B-type

1. Electronic properties of solids (3 credits)
Speaker: L. Manna
2. Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations (1 credit)
Speaker: L. de Trizio
3. Basics of Crystallography and Diffraction by crystals (1 credit)
Speaker: M. Prato
4. Introductory course on transmission electron microscopy (1 credit)
Speakers: R. Brescia, Z. Dang, J. Buha, R. Marotta 4
5. Opto-Electronic Properties of Semiconductor Quantum Dots (1 credit)
Speaker: I. Moreels
6. Spectroscopies for chemical analysis (1 credit)
Speakers: F. Palazon, R. Krahné, S. Ghosh
7. The application of Nanocrystals in energy storage, photo-catalysis and heterogeneous catalysis (1 credit)
Speakers: M. Colombo, D. Shin Shinde, S. Monaco
8. Water soluble nanoparticles (7 hours)
Speakers: T. Pellegrino
9. Synchrotrons and X-Ray Free Electron Lasers (7 h) – online course
An extensive introduction to synchrotron and X-Ray Free Electron Lasers (XFELs) facilities and associated techniques. Massive Open Online Course (MOOC) from the EPFL (Ecole Polytechnique Federale de Lausanne). (1 credit)
10. Introductory on magnetism at the nanoscale (1 credit)
Speakers: P. Guardia

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

1. "Low and Very Low Temperatures: Methods of Producing and Measuring Cryogenic Temperatures" at Unige, Speaker: I. Curlic, Department of Physics, Mathematics and Techniques, University of Prešov, Slovakia
2. "Magnetic hyperthermia : from fundamentals to biomedical applications" at the II, Speaker: F. Terán, iMdea Nanociencia, Ciudad Universitaria de Cantoblanco, 28049 Madrid, Spain
3. Nanobiotecnología, CNB-CSIC-iMdea Nanociencia, Campus Universitario de Cantoblanco, 28049, Madrid, Spain, 05/05/2016 – 06/05/2016
4. "Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials" and "Novel Materials for energy storage and conversion" at Unige Speaker: T. Fässler, Department of Chemistry Technical University of Munich, Germany, 11/05/2017
5. "An introduction to nanoscale magnetism for biomedical applications" at the IIT Speaker: N.Telling, Keele University, UK, 23/05/2017 – 24/05/2017

6. "From Crystallography to Imaging" at the IIT, Speaker: C. Giannini, Institute of Crystallography, National Research Council, Bari, Italy, 23/04/2018 – 24/04/2018

National and International Schools or Workshops

1. SPECTROCAT 2016 Laboratoire Catalyse et Spectrochimie, 27th June – 1st July 2016, Caen, Francia.
2. 4th TYC-Energy Materials Workshop: shaping Nanocatalysts 14th, December 2016 - 16th December, 2016, London
3. Catalysis Fundamentals and Practice Summer School 17th-21st July 2017, Liverpool, UK, Seminars and Courses Given (4 credits)

Seminars and Courses Given

1. Istituto Italiano di Tecnologia (IIT), Genoa (Italy), Contribution: monthly oral presentation at Catalysis Group Meeting about the progress of my activity at different stages (2015-2018).
2. Università degli Studi di Genova, Dipartimento di Chimica e Chimica Industriale (DICCI), Genoa (Italy), Date: 12/10/2016, Contribution: Oral, Title of Contribution: "Bimetallic Nanoparticles as catalyst for CO oxidation".
3. Università degli Studi di Genova, Dipartimento di Chimica e Chimica Industriale (DICCI), Genoa (Italy), Date: 13/10/2017, Contribution: Oral, Title of Contribution: "Bimetallic Nanoparticles as catalyst for CO oxidation".
4. Istituto Italiano di Tecnologia (IIT), Genoa (Italy), Date: 22/12/2017, Contribution: Oral presentation at Nanochemistry Group Meeting, Title of Contribution: "The effect of red-ox treatments on the structure and synergistic activity of PdCu and PtCu alloy catalysts for CO oxidation reaction".
5. Università degli Studi di Genova, Dipartimento di Fisica (DIFI), Genoa (Italy), Date: 13/02/2018, Contribution: Oral, Title of Contribution: "Gas atmosphere induced structural changes of bimetallic noble metal-copper nanocrystals: the role of the noble metal and the support".
6. Course "Materials Characterization at IIT"
Speaker: M. Prato, L. Pasquale, L. Ceseracciu, M. Salerno
7. Fundamentals of X-ray and Micro X-ray Fluorescence Spectroscopy 25/03/2019

Seminars Attended

1. Semiconductor Nanocrystals: Discovery, Milestones, and Recent Theoretical Developments, A. L. Efros 20/11/2015
2. Insight in the chemistry of metal sulfide nanocrystals and their application in photovoltaics, P. Reiss, 25/11/2015
3. Perovskites: an old material for the third generation of PV solar panels, L. M. Perez, 21/04/2016
4. Colloidal nanoparticles and applications, A. G. Kanaras, 28/04/2016
5. Hydration induced spin glass state in a frustrated Na-Mn-O triangular lattice, I. Bakaimi, 28/04/2016
6. Spatio-temporal visualization of atomic motions in low-dimensional materials, G. M. Vanacore, 03/05/2016
7. Ionic bonding and the effect of electron repulsion on the band structure, L. Manna 08/06/2016
8. Thermal forces: Moving and manipulating matter with thermal gradients, R. Piazza, 21/10/2016
9. Visualizing and controlling optoelectronic processes in lead halide perovskites, A. Weber-Bargioni 14/11/2016

10. Photoactive systems for solar energy conversion, luminescence and catalysis, N. Armaroli, 27/01/2017
11. Application of nanocrystals to photocatalysis and exhaust gas purification, T. Ikeda, 01/02/2017
12. Structural biopolymers – using Nature’s building blocks as an inspiration for advanced manufacturing, B. Marelli, 01/03/2017
13. Theatrocracy: the communication in the modern age, S. Amoroso, 02/03/2017
14. Synthetic methodology for colloidal nanomaterials: limitations and opportunities, D. Talapin, 26/04/2017
15. Integrated Photoelectrodes for CO₂ reduction and water oxidation, F. M. Toma, 13/06/2017
16. Perovskite nanocrystals - the new generation of defect tolerant luminescent materials, S. Sapra, 14/06/2017
17. Aberration-corrected STEM: sub-Å resolution imaging, atomic-resolution elemental mapping, and vibrational spectroscopy, O. L. Krivanek, 04/10/2017
18. Graphene and other 2D related materials interface engineering for highly efficient and stable organic and perovskite solar cells, E. Kymakis, 13/11/2017
19. Flat Optics Based on Metasurfaces, F. Capasso, 13/12/2017
20. One-Year stable perovskite solar cells by 2D/3D interface engineering, G. Grancini, 02/02/2018
21. NanoChemistry Seminar: Colloidal semiconductor nanocrystals, I. Infante, 26/02/2018 8
22. Optoelectronics Seminar: Scattering-Type Scanning Near-Field Optical Microscopy for various applications: carrier density profiling in semiconductors, plasmonic field mapping, 2D material characterization, and chemical identification of biomaterials 10 nanometer resolution, P. Schaefer, 27/02/2018
23. Overview of nanoindentation techniques and instrumentation, B. Crawford, 07/03/2018
24. Attosecond microscopy and control of matter down to the nucleus, F. Carbone, 19/10/2018
25. A New Concept of ‘Quantum’ Measurement in Transmission Electron Microscopy that Changes the Paradigm in Both TEM Material Science and Cryomicroscopy, V. Grillo, 13/02/2019

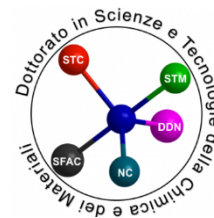
Other Activities

In situ study of structure transformations of nanoparticle catalysts:

- ROCK beamline at the SOLEIL Synchrotron (France), 22nd-25th March 2018, Research project: Gas atmosphere induced Ostwald ripening and disintegration of γ -Al₂O₃ supported bimetallic nanoparticles
- Super XAS-X10DA beamline at the Swiss Light Source (SLS) at the Paul Scherrer Institut (PSI), 5th-11st June 2018, Research project: Structure-activity relationship in noble metal-copper bimetallic nanocrystals



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



Curriculum: Nanochemistry

NICCOLÒ SILVESTRI

Start of the Doctorate Program: November 1st, 2015
End of the Doctorate Program: October 31st, 2018
Advisors: Dr. Teresa Pellegrino(IIT), Dr. Annalisa Relini(UNIGE)
Project Title: Magnetic Nanoparticles for Brain Diseases

Project abstract

The blood–brain barrier (BBB) plays an important role in protecting the brain from injury and diseases, but also restrains the delivery of potential therapeutic drugs for the treatment of brain illnesses, such neurodegenerative diseases and brain tumors. Many of that brain diseases are characterized by the deposition of β -amyloid(A β) into the extracellular matrix leading neurons to death. The most promising way to carry drugs inside the brain and act on the disease, is represented by Nanoparticles. The purpose of this research project is to engineer multimodal magnetic nanoparticles(MMNPs)in particular Iron oxide and cobalt ferrite nanocubes. TAT peptide, phosphatidic acid and hyperthermia will be used to reach the brain with a high concentration of MMNPs in order to exceed the BBB without damage. Further a specific treatment of disease will be provided using drugs and antioxidants, *e.g.*, ferulic acid or acting directly on the A β fibrils, binding them with phosphatidic acid in order to obtain a disaggregation effect. Finally the influence of hyperthermia on the fibrils linked to the particles, will be investigated as well as the possibility of enhance the BBB passage opening the tight junction with heat. The BBB will be produced *in-vitro* using endothelial cells, astrocytes and neurons following a co-culture protocol.

During this third year, I have focused my activity on the following topics:

- I. I improved the synthesis of zinc ferrite nanocubes to obtain nanoparticles of better quality.
- II. I developed the synthesis of mixed ferrite nanocubes, zinc-cobal ferrite nanocubes and manganese-cobalt ferrite nanocubes.
- III. I did the characterization of the samples (TEM, DLS, electrophoresis, ICP).
- IV. I did the magnetic characterization in water and viscous media (SAR measurements, squid and AC magnetometry).
- V. I did the relaxivity characterization (for MRI and MPI).
- VI. I cultured mouse brain endothelial cells and mouse glioblastoma cells.
- VII. I did cytoflourimetric assay to study the biocompatibility of the NCs.

ACTIVITY REPORT

Research Activity

Research Period Abroad

1. I spent two months at Lawrence Berkeley National Laboratory in the Molecular Foundry department (Berkeley California, USA), from 20th of July to 20th of September 2017. I was working on the following research project "Automatized synthesis of magnetic mixed ferrites nanocubes and anisotropic assemblies of nanocubes for magnetic hyperthermia", which is part of the CompassProject (Marie Curie Actions).
2. I spent two weeks from 9th to 23th January 2018 at the Hyperthermia Lab at iMdea Nanociencia in Madrid in the frame of a Short Term Scientific Mission funded by the COST Action RADIOMAG TD1402 on the following research project "Calorimetric and Magnetic Characterization of Different Ferrite Nanoparticles for Magnetic Hyperthermia".

The research activity was carried out at the IIT for the rest of the year.

Scientific Publications

Original publications on ISI Journals:

1. A. Sathya, P. Guardia, R. Brescia, **N. Silvestri**, G. Pugliese, S. Nitti, L. Manna, and T. Pellegrino, "Co_xFe_{3-x}O₄ Nanocubes for Theranostic Applications: Effect of Cobalt Content and Particle Size," Chem. Mater., p. acs.chemmater.5b04780, 2016.
2. Vecchione R, Quagliariello V, Giustetto P, Calabria D, Sathya A, Marotta R, Profeta M, Nitti S, **Silvestri N**, Pellegrino T, Iaffaioli RV, Netti PA, "Oil/Water nano-emulsion loaded with cobalt ferrite oxide nanocubes for photo-acoustic and magnetic resonance dual imaging in cancer: in vitro and pre-clinical studies". Nanomedicine: Nanotechnology, Biology, and Medicine (2016), doi: 10.1016/j.nano.2016.08.022

Awards:

1. Young Researcher award in recognition of best poster presentation at 12th International Summer schools "N&N: Organic Electronics & Nanomedicine" (ISSON18), 30 June-7 July 2018, Thessaloniki, Greece

Oral presentations

1. "Cobalt Ferrite NanoCubes: Synthesis, Characterization, Biocompatibility and some issues on the magnetic hyperthermia measurements", ICARO Kick off meeting ERC, Sestri Levante, June 9, 2016.
2. "Magnetic nanoparticles for brain disease", IIT Genova, October 3, 2016.
3. NABM annual group meeting, IIT Genova, June 7, 2017.
4. "Different Ferrite Nanocubes for Theranostic Applications: Synthesis, SAR Characterization and Nanobeads Formation", Inorganic Facility Meeting, LBNL Berkeley USA, September 14, 2017.
5. "Secondment report: Magnetic Nanobeads Made by Nimbus", Compass Project midterm meeting (Marie Curie Action), Camogli, Genova Italy, September 26, 2017.
6. NABM annual group meeting, IIT Genova, July, 2018.
7. "Tuning the size and the composition of ferrite nanocubes towards outstanding hyperthermia performances" 15th International conference on Nanoscience & Nanotechnologies (NN18), 5 July 2018, Thessaloniki, Greece

Poster presentations

1. "Tuning the size and the composition of ferrite nanocubes towards outstanding hyperthermia performances" 12th International Summer schools "N&N: Organic Electronics & Nanomedicine" (ISSON18), 30 June-7 July 2018, Thessaloniki, Greece

National and international schools and workshops

1. ERC "ICARO" Kick off meeting, Sestri Levante, Italy 9-10 June 2016
2. Compass project midterm meeting (Marie Curie Action), Camogli, Genova Italy, September 26, 2017.
3. 12th International Summer schools "N&N: Organic Electronics & Nanomedicine" (ISSON18), 30 June-7 July 2018, Thessaloniki, Greece

Conference attended

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

Courseware

Courses attended and passed

1. Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations (1 credit) Dr. Luca de Trizio
2. Introductory course on transmission electron microscopy (1 credit) Dr. Rosaria Brescia, Dr. Zhiya Dang, Dr. Joka Buha, Dr. Roberto Marotta
3. Opto-Electronic Properties of Semiconductor Quantum Dots (1 credit) Dr. Iwan Moreels
4. Magnetic properties and characterization techniques (1 credit) Dr. Aidin Lak
5. Electronic properties of solids (3 credits) Dr. Liberato Manna
6. Basics of Crystallography and Diffraction by crystals (1 credit) Dr. Mirko Prato
7. Spectroscopies for chemical analysis (1 credit) Dr. Francisco Palazon, Dr. Roman Krahne, Dr. Sandeep Ghosh
8. "Laboratory of Optical Fluorescence Microscopy Methods" - Dr. Marta d'Amora (3 credits)

Courses given by invited experts:

1. "Magnetic Hyperthermia: from Fundamentals to Biomedical Applications", Type A course, Dr. Francisco Teran, CNB- CSIC-iMdea (1 credit)
2. "An introduction to nanoscale magnetism for biomedical applications", Type A course, Dr. Neil Telling, Keele University (1 credit)
3. "From crystallography to imaging" Type A course, Dr. Cinzia Giannini,, CNR (1 credit)

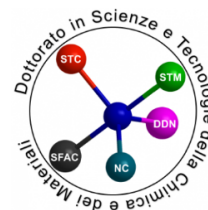
Seminars Attended:

4. "Semiconductor Nanocrystals: Discovery, Milestone, and Recent Theoretical Developments", Dr. A. L. Efros, NOV 20th, 2015.
5. "Synthesis and Chemical Manipulation of Nanoparticles for a Magnetic Improvement", Dr. V. S. S. Salgueirino, DEC 11th, 2015. .
6. "Natural Polymers of Bacterial Origin and their Medical Applications", Dr. I. Roy, DEC 18th, 2015.

7. "Perovskites: an Old Material for the Third Generation of PV Solar Panels", Dr. L.M.Perez, APR 21th, 2016.
8. 5) "NMR chemosensing with self-organized nanoparticles based receptors" Dr. F.Mancin, NOV 3rd 2017
9. "The Future of Monitoring Serotonin (and Other Neurotransmitters) in-Vivo" Dr. A.M.Andrews, MAR 20th 2017
10. "High-throughput design of doped colloidal nanocrystals" Dr. E.Chan, JUN 1st 2017
11. "From Cancer Biology to Drug Treatment: Oxaliplatin in the Era of Personalized Medicine" Dr. P.Perego, FEB 28th 2017
12. 9) "Perovskite Nanocrystals-the New Generation of Defect Tolerant Luminescent Materials" Dr. S.Sapra, JUN 13th 2017
13. "Nanoparticles and Virus" Dr.F.Stellacci, SET 22nd 2017
14. "Standardization Methods for the Synthesis of Singolcore
15. Multicore Magnetic Nanoparticles for Medical Applications" Dr.H.Gavilan, OCT 2nd 2017
16. "Fish and Grasshoppers in the Service of Mankind: exploring new in-vivo and in-vitro models" Dr. K.R.I.Olsson, OCT 4th 2017
17. "Aberration-corrected STEM: sub-Å resolution imaging, atomic-resolution elemental mapping, and vibrational spectroscopy" Dr. O.L.Krivanek, OCT 4th 2017
18. "Nanobiosensors for diagnostics applicatins" Dr.A.Merkoci, MAY 31st 2018
19. "Engineering of iron oxide nanoparticles for magnetic particle imaging guided Hyperthermia (hMPI)" Dr. A.C.Samia, JUN 6th 2018
20. "The physics of the universe, over more than 60 orders of magnitude of length" Dr. A.Ereditato, DEC 18th 2017
21. "Playing Lego at the nanoscale: Nanoparticles as building blocks for hierarchical structures" Dr.P.Guardia, DEC 11th 2017



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



Curriculum: Scienze Farmaceutiche, Alimentari e Cosmetologiche

TAPTUE GABY BRICE

Start of the Doctorate Program: *November 1st, 2015*

End of the Doctorate Program: *31st October, 2018*

Supervisor: Prof. Silvana Alfei

Thesis Title: Synthesis of amphiphilic and hydrophilic non-PAMAM dendrimers nanoparticles for biomedical applications and realization of water-soluble DDSs of twotriterpenoid acids

Thesis abstract

The purpose of my research is to prepare synthetic biodegradable non cytotoxic vectors to use in Nanomedicine, more specifically in Drug Delivery which describes the methods, formulations, technologies and systems of delivering drugs or pharmaceuticals to their site of action within an organism, with the goal of achieving a desired therapeutic effect. Researchers of our laboratory have already synthesized from 2,2-bis(hydroxymethyl)propionic acid, precursor dendrons up to the fifth generation and then biodegradable polyester dendrimers of fourth, fifth and sixth generation using 2,2-bis(hydroxymethyl)propanol as core. The prepared dendrimers functionalized with various amino acids proved non cytotoxic but poorly transfecting. During my first year of activity I was involved in the synthesis of a new generation of dendrimers functionalized with arginine and/or lysine endowed with amphiphilic character given by the introduction in the molecular structure of hydrophobic segments such as long saturated hydrocarbon chains. In this regard under the strict supervision of my supervisor I prepared the stearoyl chloride from stearic acid (C18) obtaining a mixture of mono-, di- and triester. We isolated the monostearate (44%) that was employed in a series of reactions of esterification with first and second generation dendrons obtaining two amphiphilic dendritic materials with 8 and 16 peripheral OH groups. We exploited these groups to insert protected L-arginine residues or a mixture of protected L-arginine and L-Lysine residues. Always with the help of my supervisor I adapted protocols for deprotection reactions to afford new second and third generation amphiphilic polycationic dendrimers containing 8, 16, 24 and 28 basic groups. The intermediates and the final dendrimers were all isolated, purified generally by column chromatography and characterized by IR and NMR techniques. Moreover, the final dendrimers were potentiometrically titrated to determine the buffer capacity and volumetrically titrated to determine their experimental molecular weights.

ACTIVITY REPORT

Research Activity

The research activity was carried out at the DIFAR, Department of Pharmacy, Genoa.

Scientific Publications

1. Silvana Alfei , Sara Castellaro and **Gaby Brice Taptue**. Synthesis and NMR characterization of dendrimers based on 2, 2-bis-(hydroxymethyl)-propanoic acid (bis-HMPA) containing peripheral amino acid residues for gene transfection, *Org. Commun.* (2017), 10(3), 144-177.
2. Silvana Alfei, Angela Bisio, **Gaby Brice Taptue**. Water-soluble dendrimers loaded with Ursolic and Oleanolic Acids as promising prodrugs suitable for intravenous administration, *Chinese Journal Polymer Sci.* (2018).

Communications at Conferences

Oral communications:

1. Silvana Alfei, **Gaby Brice Taptue**, "Synthesis of Arginine-Decorated Amphiphilic Dendrimers" XXXVII Conv. Naz. Div, Chimica Organica (SCI), Mestre (VE), 18-22 Settembre 2016, p. 44, OC_7.
2. Silvana Alfei, **Gaby Brice Taptue**, "New promising vectors for gene delivery by a step-wise functionalization of a polyester-based non toxic dendrimer with N,N-dimethylglycine, N-methylglycine, lysine and arginine" XXVI Conv. Naz. Della Società Chimica Italiana (SCI), Paestum (SA), 10-14 Settembre 2017, p. 189, ORG OR23.
3. Silvana Alfei, **Gaby Brice Taptue**, Angela Bisio "Water soluble polyester-based amino acids modified dendrimers loaded with ursolic and oleanolic acids as promising prodrugs suitable for intravenous administration" Giornata della Chimica Ligure, Genova, 20 Ottobre 2017, p. 15.
4. **Gaby Brice Taptue**, Silvana Alfei, Angela Bisio, "Water soluble polyester-based amino acids modified dendrimers loaded with ursolic and oleanolic acids as promising prodrugs suitable for intravenous administration" 17th Edition of the Merck Young Chemists Symposium, Milano Marittima, 13 – 15 November 2017, p. 81, OC_60.
5. Silvana Alfei, **Gaby Brice Taptue**, Sara Castellaro, "N, N, N-Tris(tert-butoxycarbonyl)-L-arginine: five isoforms whose obtainment depends on procedure and a scrupulous NMR confirmation of their structures" IX Giornate Italo-Francesi di Chimica (GIFC), Genova, 16 – 18 Aprile 2018, p. 34, OC_13.

Poster Communications:

1. Silvana Alfei, **Gaby Brice Taptue**, "Synthesis of a new dendritic amphiphilic polyester with pentaerythritol core and a multifunctional periphery for linking amino acids and for using in gene therapy", XXVI Conv. Naz. Della Società Chimica Italiana (SCI), Paestum (SA), 10-14 Settembre 2017, p. 333, PO95.
2. Silvana Alfei, **Gaby Brice Taptue**, Sara Castellaro, "How five different isoforms of N,N,N-Tris(tert-butoxycarbonyl)-L-arginine whose reactivity in esterification reactions was subsequently investigated were obtained", XXII International Conference on Organic Synthesis, 16-21 September 2018 Florence, Italy, p. 136, P9

3. Silvana Alfei, **Gaby Brice Taptue**, Sara Castellaro, "An investigation about the reactivity of five isoforms of N,N,N-Tris(tert-butoxycarbonyl)-L-arginine in esterification reactions of 1,3-propandiol Dendron derivative", XXII International Conference on Organic Synthesis, 16-21 September 2018 Florence, Italy, p. 135, P8

Congresses Attended

1. XII Congresso del gruppo interdivisionale di Chimica Organometallica (CO.GI.CO) della Società Chimica Italiana Genova, 5 - 8 Giugno 2016.
2. XXVI Congresso Nazionale della Società Chimica Italiana, Centro Congressi dell'Hotel Ariston – Paestum (SA) 10 - 14 Settembre 2017.
3. Giornata della Chimica Ligure, Difar – Genova 20 Ottobre 2017.
4. 17th Edition of the Merck Young Chemists Symposium – Milano Marittima 13 – 15 Novembre 2017.
5. IX Giornate Italo-Francesi di chimica (GIFC) – Genova 16 – 18 Aprile 2018.
6. XXII International Conference on organic synthesis – Florence 16 – 21 September 2018.

Courseware

Courses attended and passed

Courses ,Given by Teachers of the Unige and IIT:

1. "Bioorganic Chemistry" Prof. L. Banfi at DCCI, University of Genoa (2CFU)
2. "NMR Spectroscopy to characterize synthetic polymers" Prof. F. Lucchesini (DIFAR, University of Genoa) (2CFU).
3. "Innovative pharmaceutical dosage forms: preparation and control methods" Prof. Caviglioli, Prof. Baldassari, Prof. Parodi, Prof. Russo (DIFAR, University of Genoa) (2CFU).
4. "INN and IUPAC nomenclature of organic drugs" Prof. G. Grossi (DIFAR, University of Genoa) (2CFU).
5. "Principal plants used in Phytocosmetics and their constituents" Prof. A. Bisio (DIFAR, University of Genoa) (2CFU).
6. "Design and synthesis of protein-kinase inhibitors as anticancer agents" Prof. S. Schenone at DIFAR, University of Genoa (2CFU).
7. "Patent and bibliographic databases searching in medicinal chemistry" Prof. P. Fossa, Prof. C. Brullo at DIFAR, university of Genoa (2 CFU).

Courses given by invited experts:

1. "Medicinal chemistry with carbohydrates: the influenza virus and the discovery of sialidase inhibitors" Prof. Anna Bernardi, University of Milan (DCCI, University of Genoa, 13/11/2015).
2. "NIR spectroscopy: theory and applications" Dr Tiziana Cattaneo e Dr Roberto Giangiacomo (DIFAR, University of Genoa, 29/02/2016).
3. "An introduction to Nanoscale magnetism for biomedical applications" Dr. Neil Telling, Keele University, UK (IIT via Morego 30, 23/05/17 and 24/05/17)
4. "Magnetism at the nanoscale" 23/05/17
5. "Biomedical Applications of magnetic Nanoparticles" 24/05/17

6. "Superhard materials: structural chemistry of boron and borides" Prof. Peter Rogl Institute of materials chemistry and research, University of Vienna, Austria (DCCI, University of Genoa, 06/06/17 and 07/06/17)

National and International Schools or Workshops

1. International workshop on industrial waste approaches and technologies for the recovery of raw materials by complex products end of life (Genova, 17/02/2016).
2. School of Experimental Design, Section of Chemistry and Food and Pharmaceutical Technologies, Research Group of Analytical Chemistry and Chemometrics, of the Department of Pharmacy of the University of Genoa. The course took place at the Department of Economy, Aula Caffa, Via Vivaldi 5, 16126 Genoa, Prof. Riccardo Leardi September 25-29, 2017.

Seminars attended

1. "Sistema biotina-(strept)avidina nel pretargeting e in applicazioni biotecnologiche" Dott.ssa Irene Croce (DIFAR, University of Genova, 27/11/2015).
2. "Tecnologie avanzate per lo sviluppo di modelli alternativi fisiologicamente rilevanti in vitro" Dott.ssa Jenia Danailova (DIFAR, University of Genova, 27/11/2015).
3. "Reazioni palladio-catalizzate: un impatto rivoluzionario in chimica farmaceutica" Dott. Andrea Desogus (DIFAR, University of Genova, 27/11/2015).
4. "Rivoluzione nella terapia delle malattie parassitarie: Artemisinina come grande successo scientifico" Dott.ssa Cinzia M. Francini (DIFAR, University of Genova, 27/11/2015).
5. "Druglikeness e metodi di score relativi: ligand efficiency e lipophilicligandefficiency" Dott.ssa Sara Guariento (DIFAR, University of Genova, 27/11/2015).
6. "Tissue-engineering strategies to increase peripheral nerve regeneration across long gaps" Prof. Kirsten Haarstert-Talini (MedizinischeHochschule Hannover) 04/12/2015 Anfiteatro anatomico Genova.
7. "Trasmissione glutammatergica e eccitotossicità nella SLA" Prof. Giambattista Bonanno (DIFAR, University of Genova, 14/12/2015).
8. "I nutraceutici: i farmaci per le persone sane" Prof. Ettore Novellino (Dipartimento di Farmacia, Università Federico II di Napoli, 26/01/2016).
9. "Applicazioni pratiche dell'incertezza della misura in campo chimico analitico" Dr. Edoardo Tartacca (Responsabile del Laboratorio Chimico dell'Agenzia delle Dogane e dei Monopoli sede di Genova, 04/05/2016).
10. "Aspetti e prospettive della moderna industria sidurgica" Ing. Franco Belgrano(Consigliere delegato di Isositemi S.R.L, 05/05/2016).
11. "New trends in computer aided Drug Design" Dott. Tiziano Tuccinardi Ricercatore presso il Dipartimento di Farmacia dell'università di Pisa – Adjunt assistant professor presso sbarro institute for cancer research and molecular medecine center for biotechnology temple university Philadelphia, P.A USA (DIFAR, University of Genova, 18/10/16).
12. "Problematiche relative alla qualità e sicurezza delle materie prime e degli eccipienti. Tracciabilità e provenienza" Dr. Piero lamartino Vice presidente di European Industrial Pharmacists Group (viale Benedetto XV aula patologia, University of Genoa, 11/11/16).
13. "Odori, profumi e feromoni come mediatori chimici olfattivi" Dr.ssa Chiara Lacapra (DIFAR, University of Genoa, 18/11/16).

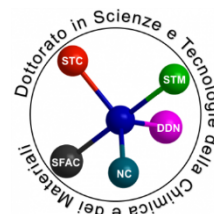
14. "Tubercolosi ed altre patologie polmonari: stato dell'arte e recenti sviluppi terapeutici" Dr. Elda Meta (DIFAR, University of Genoa, 18/11/16).
15. "Giocare sporco: PAINS e composti promiscui" Dr.ssa Anita Parricchi (DIFAR, University of Genoa, 18/11/16)
16. "Il marketing cosmetico: dalla missione aziendale alla risposta del consumatore" Dr.ssa Silvia Rum (DIFAR, University of Genoa, 18/11/16).
17. "Patient safety centre di Lipsia: una iniziativa interdisciplinare per la sicurezza del paziente" Dr. Roberto Frontini Direttore della farmacia-Università di Lipsia (Aula di patologia, University of Genoa, 31/03/17)
18. "Chemistry in the kitchen from traditional to molecular cooking" Dott.ssa Ilaria Giacchello (DIFAR, University of Genoa, 15/10/18).
19. "Oral diseases and their treatment: an overview" Dott. Kartik Neduri (DIFAR, University of Genoa, 15/10/18)
20. "Deubiquitinase inhibition as therapeutic strategy" Dott.ssa Vittoria Zoppi (DIFAR, University of Genoa, 15/10/18).

Other Activities

- Laboratory assistant in "Instrumental Analysis of drugs" (CTF) for a total of 60 hours, academic year 2016/2017.
- Laboratory assistant in "Instrumental Analysis of drugs" (CTF) for a total of 60 hours, academic year 2017/2018.



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



Curriculum: Chemical Sciences and Technologies

DANIELE URSO

Start of the Doctorate Program: *November 1st, 2015*

End of the Doctorate Program: *October 31th, 2018*

Advisors: Prof. Marina Alloisio (DCCI), Prof. Ranieri Rolandi (DIFI)

Thesis Title: Sistemi a base di chitosano per applicazioni farmacologiche

Thesis abstract

Chitosano utilizzato come Drug Delivery System per applicazioni in medicina odontoiatrica per il rilascio controllato di farmaci.

ACTIVITY REPORT

Research Activity

The research activity was mainly carried out at the Department of Chemistry and Industrial Chemistry of Unige

Scientific Publications

Original publications

1. Idrogeli di chitosano per il rilascio di farmaci in applicazioni odontoiatriche, XXII Convegno Nazionale dell'Associazione italiana di Scienza e Tecnologia delle Macromolecole, Genova 11-14 Settembre 2016 (Atti di Convegno)
2. Sistemi a base di chitosano per applicazioni farmacologiche, XXIII Convegno Nazionale dell'Associazione Italiana di Scienza e Tecnologia delle Macromolecole, Catania 9-12 Settembre 2018 (Atti di Convegno)

Communications at Conferences

Poster Communications:

1. Idrogeli di chitosano per il rilascio di farmaci in applicazioni odontoiatriche, XXII Convegno Nazionale dell'Associazione italiana di Scienza e Tecnologia delle Macromolecole, Genova 11-14 Settembre 2016
2. Sistemi a base di chitosano per applicazioni farmacologiche, XXIII Convegno Nazionale dell'Associazione Italiana di Scienza e Tecnologia delle Macromolecole, Catania 9-12 Settembre

Congresses Attended

1. XXII Convegno Nazionale dell'Associazione Italiana di Scienza e Tecnologia delle Macromolecole, Genova 11-14, Settembre 2016

Courseware

Courses attended and passed, type B courses

Courses Given by Teachers of the PhD School:

1. Corso Avanzato di Dinamica Molecolare di Proteine, Prof. Oscar Moran (Istituto di Biofisica del CNR di Genova), 3 CFU
2. Fondamenti di microscopia elettronica a scansione ed in trasmissione, Prof. Paola Riani, 3 CFU
3. Nanocompositi polimerici, Prof. Orietta Monticelli, 2 CFU
4. Composti organici per la fotonica, l'elettronica e l'optoelettronica, Prof. Davide Comoretto, 2 CFU
5. Introduzione all'applicazione della spettroscopia Raman ai materiali, Prof. Maria Carnasciali, 2 CFU
6. Caratterizzazione di nanoparticelle per mezzo della microscopia a forza atomica e Dynamic Light Scattering, Prof. Ranieri Rolandi, 2 CFU

Courses Given by invited experts, type A courses

1. Medicinal Chemistry with carbohydrates: the influenza virus and the discovery of sialidase inhibitors, Prof. Anna Bernardi (Università di Milano), 13/11/2015
2. New methods for food authenticity and safety testing, Dr. Valeria Merlo (PhD, Direzione Tecnica, Technical Manager and Director, Eurofins, Cuneo), 27/11/2015
3. Challenges in Chemical Synthesis for Energy Storage and Energy Conversion Materials, Novel Materials for energy storage and conversion, Prof. Thomas Fassler (Department of Chemistry, Technical University of Munich, Germany), 11/05/2017
- 4) Recent Advances in Computer-Aided Drug Design, Prof. Tiziano Tuccinardi (Università di Pisa), 16/10/2017
4. Chemistry and Physics of 'Materials Science of Borides and particularly of Metal Boron carbides, Prof. Peter Rogl (Università di Vienna, 11-13/06/2018

National and International Schools or Workshops

1. Summer School on Science Management for Scientists and Engineers, 6 CFU, Università di Genova, dal 10 al 21 Luglio 2017

Seminars Attended

1. Chemometrics in proteomics studies, Prof. Beata Walczak (Institute of Chemistry, Silesian University, Katowice, Poland), 22/01/2016
2. Exploring the transformation mechanisms of matter at the nanoscale with computer simulations, Prof. Fabio Pietrucci (Sorbonne Univ. – Univ. Pierre et Marie Curie, Paris), 21/11/2016

3. Sviluppo di nuovi materiali per olografia: dalla molecola al materiale, Dr. Andrea Bianco (Istituto Nazionale di Astrofisica), 03/02/2017
4. Fotopolimeri in astronomia: aspetti pratici e risultati in cielo, Dr. Alessio Zanutta (Istituto Nazionale di Astrofisica), 03/02/2017
5. Dal problema astronomico alla strumentazione: essere a metà tra scienza e tecnologia, Dr. Marco Landoni (Istituto Nazionale di Astrofisica), 03/02/2017
6. Un caso di proficua collaborazione: biocatalisi e prodotti naturali, Dr. Sergio Riva (Istituto di Chimica del Riconoscimento Molecolare, CNR Milano), 12/06/2017
7. Analisi termica accoppiata alla gas cromatografia e spettrometria di massa. Un potente strumento per la caratterizzazione dei materiali, Dr. Federico Locardi (DCCI, Università di Genova), 13/06/2017
8. Novel small molecules, targets, and strategies in anti-infective development, Prof. J.K. Sello (Brown University of Providence, USA), 03/07/2017
9. On research activities at Muroran Institute of Technology, Prof. Paolo Mele (Muroran Institute of Technology, Muroran, Hokkaido, Japan), 24/07/2017
10. Presence (PhD students as a bridge between science and society), Festival della Scienza, DCCI-Università di Genova, 27/10/2017
11. A primer to high-resolution cryo-electron microscopy, Dr. Paolo Swvec (Università Statale di Milano), 31/10/2017
12. Effect of isotactic polypropylene microstructure on crystallization and properties: the role of regiodefects, Dr. Davide Tranchida, PhD (Borealis Polyolefine GmbH), 6/12/2017
13. Ab initio simulations of phase-change materials, Prof. Riccardo Mazzarello (Institute for Theoretical Solid State Physics and JARA, RWTH Aachen, Germany), 20/12/2017
14. Investigation of biocompatible gold supports by means of Reactive Molecular Simulations, Prof. Susanna Monti (CNR-Pisa), 25/01/2018
15. Il contributo del DCCI al Programma Nazionale di Ricerche in Antartide, Prof. Marco Grot e Prof. Paola Rivaro (Università di Genova) 27/02/2018
16. Biomimetic Complex Systems for Soft Actuation and Neural Computing, Prof. Paolo Milani (CIMAINA e Dip. Fisica, Università di Milano), 10/05/2018
17. Ligands for Functional Targeting of G-Quadruplex Nucleic Acids, Prof. Mauro Freccero (Università di Pavia), 7/06/2018
18. Introduction to Shibaura Institute of Technology, Prof. Paolo Mele (SIT, Tokyo), 18/09/2018

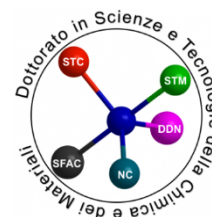
Other Activities

Corso 24 CFU per FIT:

1. Didattica della matematica
2. Metodologie e tecnologie didattiche
3. Pedagogia, pedagogia speciale e didattica dell'inclusione
4. Psicologia



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



Curriculum: Nanochemistry

MENGJIAO WANG

Start of the Doctorate Program: *November 1st, 2015*

End of the Doctorate Program: *October 31th, 2018*

Advisors: Prof. Liberato Manna (IIT); Luca De Trizio (IIT) and Ferretti Maurizio (Unige).

Thesis Title: Ru Coupled CoSe Nanocrystals with Enhanced Hydrogen Evolution Reaction

Thesis abstract

The scalable production of hydrogen could conveniently be realized by acidic water electrolysis. Currently, the major challenge confronting hydrogen evolution reaction (HER) is lacking inexpensive alternatives to platinum-based electrocatalysts. Here we report a high-efficient and stable electrocatalyst composed of CoSe NCs with a slightly amount of ruthenium (Ru). The catalysts display remarkable performance with low overpotential of only 152 mV at the current density of 10 mA/cm², and excellent stability of 80 h. Ru is the cheapest platinum-group metal and its amount in the catalyst is only 4% of atomic ratio compared to Co, showing the catalyst high activity at a very competitive price. Furthermore, a phase transformation is observed during the HER, proving that the hexagonal CoSe can be changed to orthorhombic CoSe₂ which is the real catalyst for HER. Last, a comparison of the catalysts before and after annealing was performed to prove that the annealing is helpful to improve the HER performance.

ACTIVITY REPORT

Research Activity

The research activity was mainly carried out at the IIT

Scientific Publications

Original publications on ISI Journals:

1. **Wang, M.**; Dang, Z.; Prato, M.; Shinde, D. V.; De Trizio, L.; Manna, L. Ni-Co-S-Se Alloy Nanocrystals: Influence of their Composition on their in-situ Transformation and Electrocatalytic Activity for the Oxygen Evolution Reaction. ACS Applied Nano Materials 2018.
2. Shinde, D. V.; Dang, Z.; Petralanda, U.; Palei, M.; **Wang, M.**; Prato, M.; Cavalli, A.; De Trizio, L.; Manna, L. In Situ Dynamic Nanostructuring of the Cu-Ti Catalyst-Support System Promotes

Hydrogen Evolution under Alkaline Conditions. ACS Appl Mater Interfaces 2018, 10, 29583-29592.

3. Imran, M.; Caligiuri, V.; **Wang, M.**; Goldoni, L.; Prato, M.; Krahne, R.; De Trizio, L.; Manna, L. Benzoyl Halides as Alternative Precursors for the Colloidal Synthesis of Lead-Based Halide Perovskite Nanocrystals. J Am Chem Soc 2018, 140, 2656-2664.

Communications at Conferences

Oral communications:

1. Synergistic Effect of Nickel, Cobalt, Sulfur and Selenium in the Oxygen Evolution Reaction of quaternary Ni-Co-S-Se nanocrystals. E-MRS 2018 Fall Meeting, Warsaw University of Technology, September 17-20, 2018.

Poster Communications:

1. Title: Colloidal Synthesis of Ni_{1-x}Co_xSe Nanocrystals for Electrocatalysis. ICANM2018: International Conference & Exhibition on Advanced & Nano Materials, Laval University, August 6-8, 2018.

Courseware

Courses attended and passed

1. "Electronic properties of solids"
Prof. Manna L.
3 credits.
2. "Experimental Design"
Grotti M., Leardi R.
3 credits.
3. "Nanomaterials and Nano-Heterostructures: Colloidal Synthesis and Chemical Transformations"
Dr. De Trizio L.
1 credit.
4. "Electric circuits for Electrochemistry"
Ansaldo A., Dr. Monaco S.
3 credits.
5. "Basics of Crystallography and Diffraction by crystals"
Dr. Prato M.
1 credit.
6. "Introductory course on transmission electron microscopy"
Dr. Brescia R., Dr. Marotta R., Dr. Dang Z.
1 credit.
7. "Magnetism and magnetic materials"
Dr. Lak A.
1 credit.
8. "Spectroscopies for chemical analysis"
Dr. Palazon F., Prof. Krahne R., Dr. Ghosh S.
1 credit.
9. "Energy related applications",
Dr. Colombo M., Dr. Monaco S., Dr. Shinde D.
1 credit.
10. "Opto-Electronic Properties of Semiconductor Quantum Dots"

Prof. Moreels I.

1 credit.

Courses Given by invited experts:

1. "Medicinal chemistry with carbohydrates: the influenza virus and the discovery of sialidase inhibitors", Prof. Bernardi A. (13 November, 2015, Unige) – 1 credit.
2. "Magnetic nanoparticles: from fundamentals to biomedical application", Dr. Teran F., IIT, 5, 6 June 2016 - 1 credit.

National and International Schools or Workshops

1. Summer School: Nanomaterials: Science and applications. (15-26 August, 2016, Utrecht University) – 3 credits.

Seminars Attended

1. Efros A., "Semiconductor nanocrystals: discovery, milestones and recent theoretical developments", IIT, 20 November, 2015.
2. Reiss P., "Insight in the chemistry of metal sulfide nanocrystals and their application in photovoltaics", IIT, 25 November, 2015.
3. Flatten L., "Recent advances in FIB-milled microcavities", IIT, 19 January, 2016.
4. Perez A.L., "Perovskites: an old material for the third generation of PV solar panels", IIT, 21 April, 2016.
5. Cacialli F., "The power of intermolecular interactions in organic semiconductors: from the threaded molecular wires to PCBM single crystals", IIT, 5 May, 2016.
6. Basov D. N., "Nano-photonics phenomena in van der Waal's heterostructures", IIT, 8 June, 2016.
7. Manna L. "Ionic bonding, effect of electron repulsion", IIT, 8 June, 2016.
8. Piazzia R. "Thermal forces: Moving and manipulating matter with thermal gradients", IIT, 21 October, 2016.
9. Ikeda T. "Application of Nanocrystals to photocatalysis and Exhaust Gas Purification", IIT, 1 February, 2017.
10. Beretta D. and Sanasi A. "How to characterize your semiconductor device: trends and challenges by Keysight Technologies", IIT, 9 February, 2017.
11. De Angelis F. "Interplay of Electronic and Dynamical Process in Organohalide Perovskites", IIT, 14 March, 2017.
12. Talapin D., "Synthetic methodology for colloidal nanomaterials: limitations and opportunities", IIT, 26 May, 2017.
13. Sapra S. "Perovskite nanocrystals – the new generation of defect tolerant luminescent materials", IIT, 13 June, 2017.
14. Toma F. "Integrated photoelectodes for CO2 reduction and water oxidation", IIT, 13 June, 2017.
15. Rubio H. "Standardization methods for the synthesis of single-core and multi-core magnetic nanoparticles for medical applications", IIT, 1 October, 2017.
16. Capasso F. "Flat optics based on metasurfaces", IIT, 13 December, 2017.
17. Infante I. "Colloidal semiconductor nanocrystals", IIT, 26 February, 2018.
18. Burda C. "Designing and studying perovskite materials for a renewable energy future", IIT, 5 June, 2018.
19. Carbone F. "Attosecond microscopy and control of matter down to the nucleus", IIT, 19 October 19, 2018.



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

Curriculum: Pharmaceutical, Nutritional and Cosmetic Sciences

VITTORIA ZOPPI

Start of the Doctorate Program: *November 1st, 2015*

End of the Doctorate Program: *October 31st, 2018*

Advisor: Prof. Andrea Spallarossa

Thesis Title: "Studies on iminium salts as useful reactive intermediates for the development of biologically active compounds"

Thesis abstract

The research activity of the first year of this PhD studies was carried out for two months at the University of Genoa, under the supervision of Prof. Andrea Spallarossa, and for ten months at Nerviano Medical Sciences (Milan), an Italian company involved in the research and development of breakthrough treatments for cancer, under the supervision of Dr. Eduard Felder. The research theme of this PhD program is the design, synthesis and evaluation of the biological activity of compounds of potential interest such as antineoplastic and antiviral drugs.

During the time spent at the University of Genoa, we started a study on iminium salts, useful reactive intermediates for the preparation of pharmaceutically relevant molecules. These synthons are involved in important organic reactions (e.g. Vilsmeier-Haack-Arnold, Mannich and Knoevenagel reactions) that lead to the formation of C-C bonds, undergoing rapid attack by a wide variety of nucleophiles. The aim of the project is to extend the comprehension of the reactivity of iminium salts and to develop green synthetic and work-up methodologies for the synthesis of pharmaceutically attractive compounds. To reach this goal the feasibility of the synthesis of iminium salts from different substrates (such as substituted imidazolidin-2-(thio)one, tetrahydropyrimidine-2-thione, acyclic urea and thiourea, variously substituted indoles and heterocycles) will be studied and different protocols based on green philosophy (e.g. to reduce or eliminate the use or the generation of hazardous substances to human health and the environment, avoidance waste, use alternative feedstocks and solvents) and on microwave heating will be evaluated.

At the beginning of 2016 I joined the department of Chemical Core Technologies, within Nerviano Medical Sciences, for a one-year stage, where I started a project based on PROTACs technology. PROteolysis TARgeting Chimeras (PROTAC) represent a new therapeutic strategy for drug development which promotes degradation, instead to inhibition, of target protein. PROTAC consists of a heterobifunctional compound that contains two ligands connected by a linker unit: one ligand binds to an E3 ubiquitin ligase protein, while the other ligand binds to the target protein of interest. The mechanism is based on the formation of a ternary complex (Target Protein-PROTAC-E3 ligase) which would be able to induce ubiquitination of the target protein with subsequent degradation mediated by the proteasome. This new technology could overcome some limitations associated to the "classic" protein inhibition.

The aim of the project will be the exploration of PROTACs technology against new target proteins. To reach this goal different target protein binding ligands and different linkers will be used and an *in silico* approach will be evaluated. The initial approach has been the synthesis of the published compound **DAS-6-2-2-6-CRBN** (Figure 1), developed by Crews et al., in order to confirm the proof of concept. This PROTAC contains pomalidomide, an E3 ubiquitin ligase ligand, on one end and dasatinib, a tyrosine kinase inhibitor targeting BCR-ABL, on the other end. [Angew. Chem. Int. Ed. 2015, 54, 1–5]

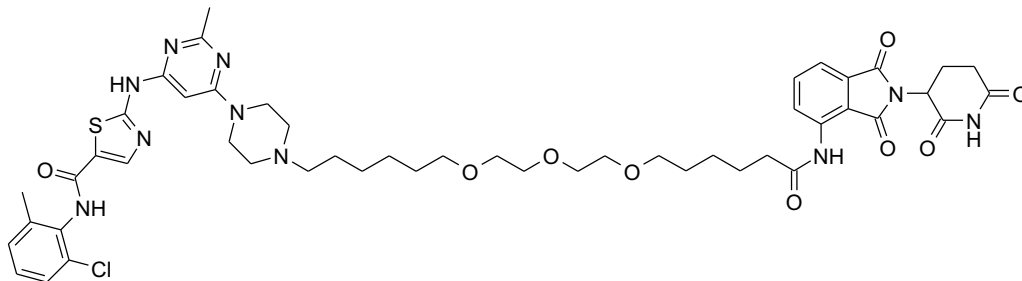


Figure 1 DAS-6-2-2-6-CRBN

In order to explore the potentiality of PROTACs, during the second part of my stage in Nerviano Medical Sciences other molecules have been synthesized and an *in silico* approach has been applied to generate a preliminary model of ABL-PROTAC-CRBN ternary complex.

My second-year activity covers the following areas:

- Synthesis of pomalidomide using a different route from that already reported last year (see Report first year) to improve NMR purity.
- Synthesis of **VZ-6-2-2-6-POMA** (Figure 2, a), **DAS-6-2-2-2-POMA** (Figure 2, b) and **DAS-6-2am-2am-6-POMA** (Figure 2, c), new PROTAC derivatives.
- *In silico* activity.

In January 2017, I joined Ciulli Lab at the University of Dundee (School of life sciences) working on the design, synthesis and biological evaluation of BRD9 PROTACs, under the supervision of Professor Alessio Ciulli. Recently, BRD9 protein, non-BET bromodomains, has gained interest as subunit of the mammalian SWI/SNF chromatin remodelling complex, mutated in the 20% of human cancer [Nat. Genet., 2013, 45, 592-601; Trends Genet., 2014, 30, 356-363]. Moreover, in literature it has been reported that BRD9 plays a role in hematopoietic cancers, supporting AML cell growth by sustaining *Myc* pathway and blocking myeloid differentiation [Nat. Chem. Bio., 2016, 12, 672-679]. Therefore, the development of molecules able to interfere with BRD9 function is of crucial relevance to understand its role in BAF complex and to exploit its potential as therapeutic target.

A library of 16 degraders has been designed, synthesized and purified to investigate the possible degradation of BRD9 *via* hijacking three different E3 ubiquitin ligase: CRL2^{VHL}, CRL4^{CRBN} and CRL4^{DCAF15}. Furthermore, all the compounds have been tested *in vitro* on different cancer cell lines (HeLa, Hek293 and U2OS cells) and immunoblotting.

During the third year of my PhD program the research activity was carried out at the University of Dundee, under the supervision of Professor Alessio Ciulli and Professor Andrea Spallarossa. The aim of the project was to further improved degradation of BRD7 and BRD9 proteins with development of VHL-recruiting PROTACs. **VZ95**, best selective BRD9 degrader developed during the second year of my PhD, was taken as template to rationally design a second generation of compounds with improved VHL-based degrader activity. Therefore, we explored the impact of varying the linkers, linkage vector, target ligand and VHL-recruiting moiety by biological characterization. The extensive structure-activity relationships (SAR) developed in this study led to the discovery of **VZ185**, a first-in-class fast, potent and selective dual degrader of BRD7 and BRD9 proteins. Relevant characteristics of **VZ185** are the rapid (apparent half-live 3.5

h) and the great degradation activity in a panel of human cancer cell lines, resulting in DC_{50} 1.76 against BRD9 and 4.5 against BRD7. Moreover, selectivity over the entire proteasome and significant antiproliferative effects were assessed. Our findings suggest **VZ185** as new chemical probe to explore the biology and therapeutic potential of degrading BRD7 and BRD9 proteins.

ACTIVITY REPORT

Research Activity

I have spent a research period in Nerviano Medical Sciences (Milan) from the 15th of January 2016 to January 14th 2017. From the 15th of January 2017 I am visiting PhD student at the University of Dundee (UK), under the supervision of Professor Alessio Ciulli.

In the last year I have won two fellowships:

- European School of Medicinal Chemistry (ESMEC, 1-5 July 2018) assigned by The Division of Medicinal Chemistry of the Italian Chemical Society
- Artificial Water Channels Faraday Discussion (25-27 June 2018, Glasgow) assigned by ScotCHEM

Scientific Publications

Original publications on ISI Journals:

1. **Zoppi** et al., Iterative design and optimization yields a potent, fast and selective PROTAC for a target-ligase pair considered unproductive to degradation, Journal of Medicinal Chemistry 2018. Manuscript submitted for publication.
2. Alfei et al., Hydrophilic and amphiphilic water-soluble dendrimer prodrugs suitable for parental administration of a non-soluble non-nucleoside HIV-1 reverse transcriptase inhibitor thiocarbamate derivative, European Journal of Pharmaceutical Sciences 2018, 124, 153-164

Communications at Conferences

Poster Communications:

1. **Zoppi V.**, Odone A., Ponassi M., Rosano C., Spallarossa A.; "Synthesis and SAR studies of novel merbarone analogues"- GIFC (Giornate Italo - Francesi di Chimica), Avignone, 25-26 April 2016.
2. **V. Zoppi**, A. Testa, C. Maniaci, S. Hughes, A. Spallarossa, A. Ciulli; "PROTACs targeting BRD7 and BRD9 subunits of BAF/PBAF complexes: design, synthesis and biological evaluation"- Presented at:
 - SLS Research Symposium, Crieff (Scotland) University of Dundee, 15-17 March 2018
 - ESMEC, Urbino, 1-5 July 2018
 - the 7th EuCheMS Chemistry Congress, Liverpool, 26-30 August 2018

Congresses Attended

1. Making Cosmetics (Milano, 25 November 2015)
2. GIFC- Giornate Italo Francesi di Chimica (Avignone, 25-26 April 2016)
3. Life cycle assessment (LCA) e sviluppo delle figure professionali: esperienze aziendali a confronto-Università degli studi di Milano (Milan, 01 Dicembre 2016)
4. SLS Research Symposium (16-18 March 2017, Crieff-Scotland)

5. SLS Scientific Trade Fair and Conference 2017 (7 May 2017, Dalhousie building, University of Dundee)
6. ACSMEDI-EFMC: Medicinal Chemistry Frontiers 2017 (23-28 June 2017, Philadelphia USA)
7. Biological Chemistry and Drug Discovery Divisional Retreat 2017 (University of Dundee, 8 December 2017)
8. SLS Research Symposium, Crieff (Scotland) University of Dundee (15-17 March 2018)
9. Artificial Water Channels Faraday Discussion, Glasgow (25-27 May 2018)
10. The 7th EuCheMS Chemistry Congress, Liverpool (26-30 August 2018)

Courseware

Courses attended and passed

1. Introduction to Project Management for Researchers, 30 May 2017 (8 hours course)
2. Introduction to research statistics for BioScience research staff and postgraduate researchers- Prof. Stephen Hubbard (16 hours) (1-2 November 2017)
3. Multiple Sequence Alignment and Analysis with Jalview- Dr Jim Procter (8 hours) (23 November 2017)
4. Kinetics, Binding & Biophysics in Drug Discovery - Walter Ward (senior enzymologist at AstraZeneca- 8 hours) (17 May 2018)
5. ScotCHEM courses (16-20 hours per course):
 - Crystallography- Prof Phil Lightfoot
 - The 'Antibiotic Apocalypse' – what can chemists do about it? - Prof Suckling
 - High-resolution NMR spectroscopy for small molecules- Dr John A. Parkinson
 - The Practice and Pitfalls of studying Organic Reaction Mechanisms- Dr Reid

Courses Given by invited experts:

1. Medicinal chemistry with carbohydrates: the influenza virus and the discovery of sialidase inhibitors (13 November 2015-Dott.ssa Anna Bernardi)
2. Taster sessions for advanced scientific technologies (School of life sciences-7.5hrs) (5 December 2017)
3. Conference and events organising- Jo Young (4 hours) (10 January 2018)
4. Division of Signal Transduction- Therapy Planning and Management Committee Meeting (8 hours) (15 May 2018)

National and International Schools or Workshops

1. XLI International Summer School in Organic Synthesis "A. Corbella"- Gargnano (BS) 12-17 Giugno 2016
2. ITC Advanced training course- Malvern, application specialist Raul Gomez, 22 May 2017 (4 hours)
3. Peptide synthesizer training course, Intavis, 25 July 2017 (4 hours)
4. European School of Medicinal Chemistry, Urbino (1-5 July 2018)

Seminars Given

1. "Studies on PROTACs: Platform Technology for Protein Degradation" - Nerviano Medical Sciences (Milan, 20 December 2016)

2. "BRD9 PROTACs: design, synthesis and biological evaluation"- University of Dundee (21 June 2017)
3. "BRD7 and BRD9 targeting PROTACs: design, synthesis and biological evaluation"- University of Dundee (5 April 2018)
4. Literature review- "Detection of Chemical Engagement of Solute Carrier Proteins by a Cellular Thermal Shift Assay" Hashimoto et al. – University of Dundee (24 May 2018)
5. "Deubiquitinase inhibition as therapeutic strategy"- Seminario XXXI ciclo, Genova (15 October 2018)

Seminars Attended

1. The Biotin-(Strept)avidin system in pretargeting and in biotechnological applications (Seminario dottorandi XXVIII ciclo; Dott.ssa Irene Croce)
2. Advanced technologies for the development of physiologically relevant in vitro alternative models (Seminario dottorandi XXVIII ciclo; Dott.ssa Jenia Danailova)
3. Palladium-catalyzed reactions: a revolutionary impact in Medicinal Chemistry (Seminario dottorandi XXVIII ciclo; Dott. Andrea Desogus)
4. Revolution in the treatment of parasitic diseases: Artemisinin as great scientific goal (Seminario dottorandi XXVIII ciclo; Dott.ssa Cinzia M. Francini)
5. Druglikeness and related scoring methods: Ligand Efficiency and Lipophilic Ligand Efficiency (Seminario dottorandi XXVIII ciclo; Dott.ssa Sara Guariento)
6. Impatto economico e sociale dell'industria farmaceutica in Italia - Farmaindustria e APHEC (Genova, 16 December 2015)
7. Natural Products Approximation for HTS Compound Libraries Design- Dr. Fabrizio Giordanetto (Università degli Studi di Genova, 22 December 2015)
8. Mechanisms of response and resistance to immune checkpoint blockade therapy in solid tumors- Dr. Andrea Anichini (Human Tumors Immunobiology Unit, Dept. of Experimental Oncology and Molecular Medicine, Fondazione IRCCS Istituto Nazionale dei Tumori, Milan) (Nerviano Medical Sciences, 12 February 2016)
9. Pd-Catalyzed Carbon-Carbon Cross Coupling Reactions and Pd-Catalyzed Carbon-Nitrogen Coupling Reactions- Professor Stephen L. Buchwald (Professor of Chemistry at MIT) (Università degli Studi di Milano, 18 April 2016)
10. From Neuroblastoma to Glioblastoma: the history of a hit-to-lead optimization – Dr. Maurizio Botta (Nerviano Medical Sciences, 19 July 2016)
11. Il marketing cosmetico: dalla mission aziendale alla risposta del consumatore- Dr.ssa Silvia Rum (Seminario XXIX ciclo SFAC, 18 November 2016)
12. Odori, profumi e feromoni come mediatori chimici olfattivi- Dr.ssa Chiara Lacapra (Seminario XXIX ciclo SFAC, 18 November 2016)
13. Giocare sporco: PAINS e composti promiscui- Dr.ssa Anita Parricchi (Seminario XXIX ciclo SFAC, 18 November 2016)
14. Tuberculosis ed altre patologie polmonari: stato dell'arte e recenti sviluppi terapeutici- Dr.ssa Elda Meta (Seminario XXIX ciclo SFAC, 18 November 2016)
15. Fragment-based approaches to probe the von Hippel-Lindau: Elongin BC complex- Dr. Guilherme Castro (University of Dundee, Division of Biological Chemistry & Drug Discovery- 1 February 2017)
16. Cryo-EM Approaches to Understanding the Eukaryotic Replisome and the Fanconi pathway for DNA repair- Dr. Alessandro Costa from The Francis Crick Institute (London) (University of Dundee, Division of Biological Chemistry & Drug Discovery- 7 February 2017)

17. VHL inhibitor as chemical probe in the hypoxia signalling pathway- Dr.ssa Julianty Frost (University of Dundee, Division of Biological Chemistry & Drug Discovery- 15 February 2017)
18. Towards computational probing of protein surfaces- Dr. Xavier Lucas (University of Dundee, Division of Biological Chemistry & Drug Discovery- 15 February 2017)
19. Mechanisms for cellular AMPK activation and glucose sensing- Professor Sheng-Cai Lin, School of Life Sciences Xiamen University, China (University of Dundee- 22 February 2017)
20. Antivirals a lot has been achieved yet a long way to go- Professor Johan Neyts (University of Leuven (Belgium), 8 March 2017)
21. Adventures in Cardiovascular drug discovery: Drug discovery without HTS screening-Paul Willis (Medicines for Malaria Venture) (9 March 2017)
22. To design and develop chemistry to make novel high quality fragments- Nicola Luise (University of Dundee) (15 March 2017)
23. A structural exploration of t-RNA synthetases as drug targets- Chimed Jansen (Division of Biological Chemistry & Drug Discovery, University of Dundee) (22 March 2017)
24. Screening of the in-house fragment library against the highly validated Mycobacterium Tuberculosis target InhA- Dan Fletcher (Division of Biological Chemistry & Drug Discovery, University of Dundee) (22 March 2017)
25. Recent Development of Proteolysis Targeting Chimera- Dr Kwok-Ho Chan (Division of Biological Chemistry & Drug Discovery, University of Dundee) (19 April 2017)
26. Towards Validation of FAN-1 as a Cancer Target- David Foley (Division of Biological Chemistry & Drug Discovery, University of Dundee) (19 April 2017)
27. Protein glycosylation: structures and functions of potential antivirulence targets- Professor Barbara Imperiali, Massachusetts Institute of Technology (4 May 2017)
28. Regulation of inflammation by TPL-2 kinase- Dr Steve Ley (Francis Crick Institute - Mill Hill Laboratory) (17 July 2017)
29. Lysyl tRNA Synthetase as a target for Kinetoplastid Drug Discovery- Peter Dodd (13 September 2017, Division of Biological Chemistry & Drug Discovery, University of Dundee);
30. Fluoro-Hydroxyprolines: synthesis, conformational analysis and binding to VHL protein- Dr Andrea Testa (13 September 2017, Division of Biological Chemistry & Drug Discovery, University of Dundee)
31. Parkin-mediated ubiquitination of the pro-apoptotic protein BAK- Dr Jon Bernardini (Walter and Eliza Hall Institute – Melbourne, Australia- 25 September 2017)
32. Tackling kinase inhibitor resistance: from cancer biology to patient outcomes- Dr Paul Huang, Institute of Cancer Research (ICR), London, (2 October 2017)
33. Protein-Protein Interactions and small molecule targeting of the multisubunit SOCS2-EloBC-Cul5-Rbx2 E3 ubiquitin ligase- Wei-wei Kung (Division of Biological Chemistry & Drug Discovery, University of Dundee) (15 November 2017)
34. Anticancer Sulfonamides Induce Selective Protein Degradation of Splicing Factor CAPERalpha (RBM39)- Dr. Takashi Owa (Chief Discovery Officer of Eisai Oncology Business Group) (29 November 2017)
35. Defining D-arabinose metabolism in *L. major* and *C. fasciolute*- Elda Iljazi (PhD Viva-Division of Biological Chemistry & Drug Discovery, University of Dundee) (15 January 2018)
36. Optimising a 'Bump-&-Hole' Approach for Selective BET Bromodomain Inhibition-Andrew Runcie (Division of Biological Chemistry & Drug Discovery, University of Dundee) (24 January 2018)
37. Shorten TB Programme: MMV46 from Hit to Lead- Kirsteen Green (Division of Biological Chemistry & Drug Discovery, University of Dundee) (7 February 2018)

38. Nuclear Lamina. Insights from Trypanosomes- Norma Padilla-Mejia (Division of Biological Chemistry & Drug Discovery, University of Dundee) (7 February 2018)
39. Immuno-Oncology: Looking beyond T lymphocytes- Dr Yumeng Mao, AstraZeneca, Cambridge, UK (27 February 2018)
40. Cryo-EM studies of the proteasome: from function to drug design- Dr Paula de Fonseca, Cambridge (27 February 2018)
41. RNMT: A Tale of two Constructs- Dr Lesley-Anne Pearson (Division of Biological Chemistry & Drug Discovery, University of Dundee) (9 May 2018)
42. Structural characterization of VCB-PROTAC ternary complexes- Dr Scott Hughes (Division of Biological Chemistry & Drug Discovery, University of Dundee) (9 May 2018)
43. Small-molecule approaches to interrogate the druggability of the VHL E3 Cullin RING Ubiquitin Ligase- Pedro Soares (PhD Viva) (16 May 2018)
44. New Photoredox Reactions- Professor David MacMillan, Princeton University (University of St. Andrews) (29 May 2018)
45. Nanoluc luciferase- derived tools for drug discovery: new ways to monitor PROTAC-Induced protein degradation and target engagement in living cells- Dr Craig Malcom (Promega) (7 June 2018)
46. Protein-protein interaction and small molecule targeting of the multisubunit SOCS2-EloBC-Cul5-Rbx2 E3 ubiquitin ligase- Wei-Wei Kung (PhD Viva) (14 June 2018)
47. Using targeted, multiplexed proteomics to understand Ubiquilins- Dr Alexandra Whiteley (Harvard Medical School) (16 August 2018)
48. The CRL4 ubiquitin ligase: at the intersection *of genome stability and drug discovery*- Dr Nicolas Thoma (Friedrich Miescher Institute (FMI), Basel Switzerland) (21 August 2018)
49. To Design and Develop Semi-saturated and Unsaturated Bicyclic Heterocycles for Fragment-Based Drug Discovery (FBDD) Campaigns- Nicola Luise (PhD Viva) (27 September 2018)

Other Activities

Corsi di formazione: Salute e Sicurezza sul lavoro, settore M 72 Ricerca scientifica e sviluppo (72.19.09)

- Formazione generale (4 ore, on-line, 2-10/03/2016)
- Formazione specifica (12 ore, presso Nerviano Medical Sciences, 6-20/07/2016)
- Formazione specifica dei lavoratori (2 ore, presso Nerviano Medical Sciences, 24/05/2016)