



Società Chimica Italiana

***Atti del
XXVI Congresso Nazionale
della Società Chimica Italiana***

Centro Congressi Hotel Ariston
Paestum (SA), 10-14 settembre 2017

Vol I

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SOMMARIO

XXVI Congresso Nazionale della Società Chimica Italiana	4
Comitato Scientifico	4
Comitato Organizzatore	4
Segreteria Organizzativa.....	5
Programma Scientifico.....	6
▪ Domenica 10 Settembre 2017.....	6
▪ Lunedì 11 Settembre 2017.....	6
▪ Martedì 12 Settembre 2017.....	7
▪ Mercoledì 13 Settembre 2017	8
▪ Giovedì 14 Settembre 2017	9
Medaglie della Società Chimica Italiana.....	11
Conferenze delle Medaglie SCI	13
▪ Light, chemistry and energy: a 20-year journey across sustainable concepts and approaches	14
▪ Solar-driven chemistry and solar fuels: the next revolution	15
▪ "There are no evil molecules" Education and dissemination for a mitigation of "bad" Chemistry	16
▪ From the Marotta's Institute to Sapienza University passing through Camerino: Sixty years spent working in the field of chemistry.	17
▪ Far comprendere la chimica per fare amare la chimica Elogio della didattica.....	18
▪ Solid state quantum chemistry: towards the rational design of nano- and photo-catalysts.....	19
▪ Polymers and Polymeric Composites for Flexible Opto-Electronic Devices	20
▪ Exploring the cytotoxic, apoptotic and antitumoral effects of two new gold N-heterocyclic carbene-gold(I) complexes on A2780 human ovarian cancer cells	21
▪ Tumor Targeting with Integrin Ligand - Drug Conjugates.....	22
▪ Can chemistry replace the scalpel? The case of photodynamic therapy.....	23
▪ Towards the Greening of Oxidation Reactions.....	25
Speaker Invitati	26
Conferenze Plenarie	28
▪ Environmental Chemistry: Quo Vadis?.....	29
▪ The chemistry of Pigment Degradation: Investigations at different Length Scales.....	30
▪ Mixed-Anion Semiconductor Photocatalysts for Visible Light Induced Water Splitting	31
▪ Towards the reprogramming of cancer cells with chemical tools targeting DNA methylation	32
▪ Advanced instrumentation for the astronaut health monitoring and diagnostics during long-term space exploration.....	33
▪ Lessons from enzymes - On the role of steric constraints and chemical environments for catalysis.....	34
▪ The catalytic production of chemicals from waste bio-oils.....	35
Keynote e Conferenze su Invito	36
▪ From a Linear to a Circular Economy The Role of Energy	37
▪ The Versatility of Mesoscopic Solar Cells	38
▪ Critical materials and the circular economy European actions and opportunities.....	39
▪ Of Prions and Other Tales.....	40
▪ Seeing, Measuring and Understanding Vesicular Exocytosis of Neurotransmitters with Micro- and Nanoelectrodes	41
▪ Organic Synthesis Goes Flow - The Use of Continuous Flow Technology for the Synthesis of Active Pharmaceutical Ingredients.....	42
▪ How will Green Chemistry Influence the Future?	43
▪ Marine organic aerosol in Marine Boundary Layer	44
▪ Lies, damned lies: detecting forgeries and manipulations in published scientific images.....	45
▪ Overview of the R&D program at Eni	46
Sessione del Gruppo Senior: <i>Chimica e Sport</i>.....	47
▪ Doping-Antidoping and the Role of the Bio-medicolegal Sciences.....	48
▪ The great changes in the 4 th industrial revolution.....	49
Grafene e Sue Possibili Applicazioni Industriali	50
▪ Second and third generation graphenes for energy conversion	51
▪ CVD graphene: transparency, conductivity and flexibility,	52
▪ Facile and sustainable functionalization method for preparing graphene layers with different solubility parameters	53

▪ Continuous flow synthesis of functionalized graphene	54
▪ Functionalization and applications of graphene-based materials	55
▪ Black Phosphorus: from Ugly Duckling to Black Swan	56
▪ Tailored polysulfone-graphene oxide adsorbers for water remediation	58
▪ New Applications of Oxidized Nanocarbons: from Catalysis to Nanocomposites	59
▪ Vibrational spectroscopy investigations on graphene/Poly (lactic acid) composites.....	60
▪ Porous graphene-based polyurethane foams-aerogel composites prepared via unidirectional freeze-drying process.....	61
▪ Multifunctional properties of Graphene Nanoplatelets based nanolaminates	62
Formulazioni nell'Industria Chimica e Farmaceutica	64
▪ Formulation and Specialty Chemistry: the needs of Chemical Industries	65
▪ Formulation challenges and emerging technologies in the pharmaceutical industry: an overview	66
▪ Formulation Chemistry: a new frontier of the Chemistry in Italy	67
▪ Trimbow® a new extrafine triple combination in a single inhaler for COPD treatment	68
▪ Study of the nanostructure of innovative formulations for cement mixtures	69
▪ Innovative approaches to tailor a particle size distribution	70
▪ I cosmetici per pelli sensibili: strategie formulative per la modulazione dell'attività lenitiva ed anti-infiammatoria.....	71
▪ Challenges in formulating Ace Bleach products	72
▪ Formulazioni nel settore della nutraceutica: stato dell'arte e prospettive future	73
▪ Colloids and Nanosciences: Formulations and New Challenges.....	74
▪ Polysaccharides based in situ gelling powders as promising wound healing medical devices.....	75
▪ Industrial Formulation: a new curriculum in Industrial Chemistry Master's degree	76
Elenco degli Autori	77
Elenco dei Partecipanti	79

XXVI CONGRESSO NAZIONALE DELLA SOCIETÀ CHIMICA ITALIANA

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- Cristina Pastore Logistica e organizzazione locale
- ZON Service sas Sito Web SCI 2017

Programma Scientifico

Domenica 10 Settembre 2017

<i>Centro Congressi dell'Hotel Ariston - Paestum</i>	
10:00-14:00	Registrazione
<i>Auditorium Giove</i>	
14:30-15:00	<i>Cerimonia di Apertura del XXVI Congresso Nazionale SCI</i>
15:00-15:30	<i>Cerimonia di Conferimento delle Medaglie SCI</i>
Sessione Plenaria - Plenary Session <i>Chimica per la tutela dell'ambiente e del patrimonio culturale</i> <i>Chemistry for environmental protection and for preservation of cultural heritage</i>	
<i>Auditorium Giove</i>	
Chairperson: Fabrizio Passarini	
15:30-16:10	GEN PL01 - Martin Scheringer <i>Environmental Chemistry: Quo Vadis?</i>
16:10-16:30	GEN IL01 - Maria Cristina Facchini <i>Marine organic aerosol in Marine Boundary Layer</i>
16:30-16:50	GEN MD01 - Tiezzi SCI Medal Lecture - Nicola Armaroli <i>Light, chemistry and energy: a 20-year journey across sustainable concepts and approaches</i>
16:50-17:20	Coffee Break
Chairperson: Lucia Toniolo	
17:20-18:00	GEN PL02 - Koen Janssens <i>The chemistry of Pigment Degradation: Investigations at different Length Scales</i>
18:00-18:30	GEN MD02 - Cannizzaro SCI Medal Lecture - Gabriele Centi <i>Solar-driven chemistry and solar fuels: the next revolution</i>
18:30-18:50	GEN MD03 - Marotta SCI Medal Lecture - Matteo Guidotti <i>There are no evil molecules. Education and dissemination for a mitigation of "bad" Chemistry</i>
18:50-19:10	GEN MD04 - Marotta SCI Medal Lecture - Domenico Misiti <i>From the Marotta's Institute to Sapienza University passing through Camerino: Sixty years spent working in the field of chemistry</i>
19:10-19:30	GEN MD05 - Illuminati SCI Medal Lecture by Fabio Olmi <i>Far comprendere la chimica per fare amare la chimica-Elogio della didattica</i>
<i>Sala Giunone</i>	
20:30-22:30	Evento sociale: Party di benvenuto – Social event: Welcome party

Lunedì 11 Settembre 2017

Sale delle Divisioni presso Centro Congressi Hotel Ariston e Hotel Savoy	
9:00-10:30	<i>Lavori delle Divisioni (consultare i programmi delle Divisioni)</i>
10:30-11:00	Coffee Break
11:00-13:00	<i>Lavori delle Divisioni (consultare i programmi delle Divisioni)</i>
13:00-14:00	Intervallo Pranzo – Lunch Break
Sala Paestum B Centro Congressi Hotel Ariston	
14:00-15:00	Sessione Poster I (consultare i programmi delle Divisioni)
Sale delle Divisioni presso Centro Congressi Hotel Ariston e Hotel Savoy	
15:00-16:30	<i>Lavori delle Divisioni (consultare i programmi delle Divisioni)</i>
16:30-17:00	Coffee Break
17:00-18:30	<i>Lavori delle Divisioni (consultare i programmi delle Divisioni)</i>
18:30-20:00	Assemblee generali delle Divisioni presso sale Hotel Ariston

<i>Giardini e Terrazze Hotel Ariston</i>	
20:00-21:00	<i>Evento sociale: Aperitivo serale</i>

<i>Auditorium Giove</i>	
21:00-21:30	GEN IL02 Conferenza serale su Etica e Scienza - Enrico Bucci <i>Lies, damned lies: detecting forgeries and manipulations in published scientific images</i>

Martedì 12 Settembre 2017

<i>Sale delle Divisioni presso Centro Congressi Hotel Ariston e Hotel Savoy</i>	
9:00-10:30	<i>Lavori delle Divisioni (consultare i programmi delle Divisioni)</i>
10:30-11:00	Coffee Break
11:00-13:00	<i>Lavori delle Divisioni (consultare i programmi delle Divisioni)</i>
13:00-14:00	Intervallo Pranzo – Lunch Break
<i>Sala Paestum B Centro Congressi Hotel Ariston</i>	
14:00-15:00	<i>Sessione Poster 2 (consultare i programmi delle Divisioni)</i>
<i>Auditorium Giove</i>	
Sessione Plenaria-Plenary Session: Chimica per l'economia circolare - Chemistry for circular economy	
Chairperson: Vincenzo Barone	
15:00-15:30	GEN KN01 Vincenzo Balzani <i>From a Linear to a Circular Economy. The Role of Energy</i>
15:30-16.10	GEN PL03 ChemPubSoc Europe Lecture - Ryu Abe <i>Mixed-Anion Semiconductor Photocatalysts for Visible Light Induced Water Splitting</i>
16:10-16:30	GEN MD06 Pisani SCI Medal Lecture - Gianfranco Pacchioni <i>Solid state quantum chemistry: towards the rational design of nano- and photo-catalysts</i>
16:30-17:00	Coffee Break
Chairperson: Alessandro Abbotto	
17:00-17:30	GEN KN02 Anders Hagfeldt <i>The Versatility of Mesoscopic Solar Cells</i>
17:30-18:00	GEN KN03 David Peck <i>Critical materials and the circular economy. European actions and opportunities</i>
18:00-18.30	GEN MD07 Natta SCI Medal Lecture - Antonio Facchetti <i>Polymers and Polymeric Composites for Flexible Opto-Electronic Devices</i>
<i>Auditorium Giove</i>	
18.30-20.00	<i>Assemblea Generale dei Soci della Società Chimica Italiana</i>
<i>Sala Giunone</i>	
20.30	<i>Evento sociale – Social event: Cena Cilentana - Typical local dinner</i> <i>“Cerimonia di consegna del Premio SCI-Reaxys” Elsevier</i>

Mercoledì 13 Settembre 2017

<i>Auditorium Giove</i>	
Sessione Plenaria - Plenary Session: Chimica per la salute - Chemistry for health	
Chairperson: Roberto Fattorusso	
9:00-9:40	GEN PL04 Paola Arimondo <i>Towards the reprogramming of cancer cells with chemical tools targeting DNA methylation</i>
9:40-10:10	GEN KN04 Giuseppe Legname <i>Of Prions and Other Tales</i>
10:10-10:30	GEN MD08 Bertini SCI Medal Lecture by Chiara Gabbiani <i>Exploring the cytotoxic, apoptotic and antitumoral effects of two new gold N-heterocyclic carbene-gold(I) complexes on A2780 human ovarian cancer cells</i>
10:30-11:00	Coffee Break
Chairperson: Francesco Paolucci	
11:00-11:40	GEN PL05 Aldo Roda <i>Advanced instrumentation for the astronaut health monitoring and diagnostics during long-term space exploration</i>
11:40-12:10	GEN KN05 Christian Amatore <i>Seeing, Measuring and Understanding Vesicular Exocytosis of Neurotransmitters with Micro- and Nanoelectrodes</i>
12:10-12:30	GEN MD09 Piria SCI Medal Lecture by Cesare Gennari <i>Tumor Targeting with Integrin Ligand - Drug Conjugates</i>
12:30-13:00	GEN MD10 Avogadro SCI Medal Lecture by Nino Russo <i>Can chemistry replace the scalpel? The case of photodynamic therapy</i>
13:00-14:00	Intervallo Pranzo – Lunch Break
Sala Paestum B Centro Congressi Hotel Ariston	
14:00-15:00	Sessione Poster 3 (consultare i programmi delle Divisioni)
Sale delle Divisioni presso Centro Congressi Hotel Ariston e Hotel Savoy	
15:00-16.30	Lavori delle Divisioni (consultare i programmi delle Divisioni)
16:30-17:00	Coffee Break
17.00-18.30	Lavori delle Divisioni
Sessione del Gruppo Senior: Chimica e Sport Senior Group Session: Chemistry and Sport	
Sala Diana	
Chairperson: Domenico Misiti	
15:00-15:30	GRS IL01 Santo Davide Ferrara <i>Doping-Antidoping e ruolo delle Scienze Biomedicolegali</i>
15:30-16:00	GRS IL02 Luigi Nicolais <i>I grandi cambiamenti nella 4° rivoluzione industriale</i>
16:30-17:00	Coffee Break
Chairperson: Rosario Nicoletti	
17.00-17.30	Aracne Editrice – Comitato Editoriale SCI <i>Presentazione della Collana “Molecole in primo piano”</i>
	Assemblea Gruppo Senior SCI
Sala Giunone	
20:30	Cena Sociale – Social Dinner

Giovedì 14 Settembre 2017

<i>Auditorium Giove</i>	
Sessione Plenaria - Plenary Session: Produzione sostenibile e sviluppo economico Sustainable production and economic development	
Chairperson: Vittorio Maglia	
9:00-9.20	<i>Introduction by Chairperson</i> "Mario Giacomo Levi Award" ceremony, a prize of the Division of Industrial Chemistry sponsored by Federchimica in recognition of a public-private joint research project developed at industrial level
9.20-10:00	GEN PL06 Johannes A. Lercher <i>Lessons from enzymes - On the role of steric constraints and chemical environments for catalysis</i>
10:00-10:30	GEN KN06 Oliver Kappe <i>Organic Synthesis Goes Flow - The Use of Continuous Flow Technology for the Synthesis of Active Pharmaceutical Ingredients</i>
10:30-11:00	Coffee Break
Chairperson: Adriana Saccone	
11:00-11:30	GEN KN07 Paul T. Anastas <i>How will Green Chemistry Influence the Future?</i> "Primo Levi Award" ceremony, a prize of the SCI Junior Group
11:30-11.50	GEN IL03 Francesca Ferrazza <i>Overview of the R&D program at Eni</i>
11:50-12:10	GEN MD11 Paternò SCI Medal Lecture by Giorgio Strukul <i>Towards the Greening of Oxidation Reactions</i>
12:10-12:50	GEN PL07 David Cole-Hamilton <i>The catalytic production of chemicals from waste bio-oils</i>
12:50-13:10	<i>Cerimonia di Chiusura – Closing Ceremony</i>
13:10-14:30	Intervallo Pranzo-Lunch Break

Eventi satellite di interesse industriale Satellite events of industrial interest	
<i>Auditorium Giove</i>	
14:30-18:00	<i>Grafene e sue possibili applicazioni industriali Graphene and its possible industrial applications</i>
Chairperson: Vincenzo Palermo	
14:30-14:45	ESG IL01 Gaetano Granozzi <i>Second and third generation graphenes for energy conversion</i>
14:45-15:00	ESG IL02 Giovanni Bruno <i>CVD graphene: trasparency, conductivity and flexibility, three inseparable properties to develop innovative applications</i>
15:00-15:15	ESG IL06 Maurizio Peruzzini <i>Black Phosphorus: from Ugly Duckling to Black Swan</i>
15:15-15:30	ESG IL04 Michele Maggini <i>Continuous flow synthesis of functionalized graphene</i>
15:30-15:45	ESG IL05 Zhenyuan Xia <i>Functionalization and applications of graphene-based materials</i>
15:45-16:00	ESG IL03 Maurizio Galimberti <i>Facile and sustainable functionalization method for preparing graphene layers with different solubility parameters</i>
16:00-16:30	Coffee Break
Chairperson: Gaetano Guerra	

16:30-16:45	ESG IL07 Manuela Melucci <i>Tailored polysulfone-graphene oxide adsorbers for water remediation</i>
16:45-17:00	ESG IL08 Maria Rosaria Acocella <i>New Application of Oxidized Nanocarbons: from Catalysis to Nanocomposites</i>
17:00-17:15	ESG IL09 Pellegrino Musto <i>Vibrational spectroscopy investigations on graphene/Poly(lactic acid) composites</i>
17:15-17:30	ESG IL10 Marino Lavorgna <i>Porous graphene-based polyurethane foams-aerogel composites prepared via unidirectional freeze-drying process</i>
17:30-17:45	ESG IL11 Michele Giordano <i>Multifunctional properties of Graphene Nanoplatelets based nanolaminates</i>

Sala Mercurio	
14:30-18.00	Formulazioni nell'industria chimica e farmaceutica Formulations in the Chemical and Pharmaceutical Industry
Chairperson: Gerardino D'Errico, Martino Di Serio	
14:30-14:35	<i>Introduction by Chairperson</i>
14:35-14:50	ESF IL01 Vittorio Maglia <i>Chimica delle formulazioni e chimica delle specialità: le esigenze dell'industria</i>
14.50-15:05	ESF IL02 Marco Adami <i>Formulation challenges and emerging technologies in the pharmaceutical industry: an overview</i>
15:05-15:20	ESF IL03 Sesto Viticoli <i>I formulati, nuova frontiera della chimica italiana</i>
15:20-15:35	ESF IL04 Enrico Zambelli <i>Trimbow® a new extrafine triple combination in a single inhaler for COPD treatment</i>
15:35-15:50	ESF IL05 Giorgio Ferrari <i>Studio della struttura alla scala nanometrica di formulati cementizi</i>
15:50-16:05	ESF IL06 Salvatore Mercuri <i>Innovative approaches to tailor a particle size distribution</i>
16:05-16:30	Coffee Break
Chairperson: Rita Patrizia Aquino, Gianluca Sbardella	
16:30-16:45	ESF IL07 Franco Gasparri <i>I cosmetici per pelli sensibili: strategie formulative per la modulazione dell'attività lenitiva ed anti-infiammatoria</i>
16:45-17:00	ESF IL08 Stefano Resta <i>Challenges in formulating Ace Bleach products</i>
17:00-17:15	ESF IL09 Antonino Bagnulo <i>Formulazioni nel settore della nutraceutica: stato dell'arte e prospettive future</i>
17:15-17:30	ESF IL10 Massimo Bonini <i>Colloidi e Nanoscienze: Formulazioni e nuove sfide</i>
17:30-17:45	ESF IL11 Pasquale Del Gaudio <i>Polysaccharides based in situ gelling powders as promising wound healing medical devices</i>
17:45-18:00	ESF IL12 Martino Di Serio <i>Formulazioni industriali, un nuovo indirizzo di laurea</i>

Medaglie della Società Chimica Italiana

Medaglia Amedeo Avogadro 2017

Nino Russo **Università della Calabria**

“come riconoscimento ad una carriera spesa a favore dell’avanzamento di conoscenze metodologiche della chimica computazionale e della formazione di nuove generazioni di giovani ricercatori nello stesso ambito disciplinare”

Medaglia Stanislao Cannizzaro 2017

Gabriele Centi **Università di Messina**

“per il grande contributo allo sviluppo di processi chimici nella prospettiva di un utilizzo efficiente e sostenibile delle risorse materiali ed energetiche”

Medaglia Giulio Natta 2017

Antonio Facchetti **Northwestern University and Flexterra Inc.**

“per l’eccezionale valore scientifico e l’innovatività della ricerca su temi di grande attualità, quale lo sviluppo di dispositivi macromolecolari per applicazioni elettroniche, condotta in Italia ed all’estero”

Medaglia Ivano Bertini 2017

Chiara Gabbiani **Università di Pisa**

“per i brillanti e innovativi risultati ottenuti nella ricerca in chimica farmaceutica e bioinorganica”

Medaglia Gabriello Illuminati 2017

Fabio Olmi

“per il continuo e qualificato impegno, sia scientifico che istituzionale, nel campo della Didattica della Chimica”

Medaglie Domenico Marotta 2017

Matteo Guidotti **CNR-Istituto di Scienze e Tecnologie Molecolari**

“per la sua attività di divulgazione e di impegno civile, condotta con generosità ed entusiasmo”

Domenico Misiti **“Sapienza” Università di Roma**

“per l’incessante lavoro svolto a favore della comunità chimica tutta in importanti istituzioni nazionali ed organizzazioni internazionali”

Medaglia Emanuele Paternò 2017

Giorgio Strukul **Università di Venezia**

“per la capacità di indirizzare la sua ricerca su sistemi catalitici omogenei ed eterogenei alla sostenibilità ed allo sviluppo di nuove metodologie”

Medaglia Raffaele Piria 2017

Cesare Gennari Università di Milano

“per il fondamentale e innovativo contributo dato alla chimica organica con le sue ricerche nel campo della catalisi omogenea e della bioorganica”

Medaglia Cesare Pisani 2017

Gianfranco Pacchioni Università di Milano Bicocca

“per i suoi straordinari risultati ottenuti nell’applicazione del calcolo ad una molteplicità di studi su materiali nanostrutturati e loro superfici”

Medaglia Enzo Tiezzi 2017

Nicola Armaroli CNR Istituto per la Sintesi Organica e la Fotoreattività,

“per la grande visibilità e autorevolezza scientifica conquistato a livello nazionale e internazionale sui complessi temi della sostenibilità energetica e ambientale nella loro più vasta accezione”

Conferenze delle Medaglie SCI

Light, chemistry and energy: a 20-year journey across sustainable concepts and approaches

Nicola Armaroli

*Istituto per la Sintesi Organica e la Fotoreattività, Consiglio Nazionale delle Ricerche (ISOF-CNR)
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The investigation of fundamental phenomena in photochemistry and photophysics (*e.g.*, energy transfer, electron transfer, luminescence) is a privileged path to explore a variety of molecules, supermolecules and materials of wide (and sometimes unexpected) interest in the area of sustainable chemistry. In this lecture, I will give an overview of some key findings of my research over 20 years, outlining future perspectives. I will focus in particular on carbon nanomaterials for solar energy conversion (1-3), luminescent complexes and materials for lighting devices (4,5) and photocatalysis (6), copper complexes as alternatives to related materials based on rare and expensive elements (7). Key bottlenecks on the path of the energy transition from fossil fuels to renewables will also be highlighted (8).

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Solar-driven chemistry and solar fuels: the next revolution

Gabriele Centi and Siglinda Perathoner

^a Univ. Messina, ERIC aisbl and INSTM/CASPE, Industrial Chemistry (Dept.s MIFT & ChimBioFarAm),
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Driven from competitiveness in a changing economic world with an increasing transition to renewable energy, chemical and refinery production are in a major transition phase to go beyond fossil fuels (as main raw materials and energy source) and to increase sustainability. It is thus necessary to rethink chemical and refinery production methodologies from this perspective, with consequent need of new approaches to chemical industrial production (1). Between the emerging hot areas are those generally indicated as solar-driven chemistry and solar fuels (2).

Solar-driven chemistry indicates the general effort to develop the sustainable chemistry of the future based on the progressive decrease of the massive use of fossil fuels and the introduction of renewable energy in the value chain. It is thus a new vision for sustainable chemical (and energy vectors) production, and has a major impact on catalysis and process engineering. In fact, moving from the use of thermal energy (as currently in most of chemical processes) to the use of photon, electrons, radiations, etc., as necessary for addressing the challenge of solar-driven chemistry, requires to conceptually redesign catalysis and industrial processes. Solar fuel is the parallel concept of energy vectors which are able to convert renewable energy sources (with all the associated problems of discontinuity, transport, etc.) to chemical energy vectors which allow to trade on a world scale energy, as actually made for fossil fuels, but base on renewable energy sources (3).

The key issue is to use renewable energy (photons, electrons, radiations) rather than thermal energy (deriving from fossil fuels, as currently in over 98% of industrial cases) to drive chemical production (4). While there is still large skepticism or at least seen as a very-long-term objective, this lecture will try to evidence how the transition is instead on a relatively short-term, with identification of the possibilities, and challenges to address, and the identification of a new possible chemical production tree to create the future low-carbon chemical production, with a minimized use of fossil fuels and the progressive introduction of new routes for the production of large-volume chemicals or intermediates.

This lecture will include in the discussion also some of the areas on which we are working, like the electrochemical conversion of CO₂ to acetic acid (5) or to produce ethylene glycol, or of N₂ conversion to NH₃ (6).

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“There are no evil molecules” Education and dissemination for a mitigation of “bad” Chemistry

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“There are no bad molecules, only evil human beings” is a famous sentence by Roald Hoffmann (1), Nobel laureate in Chemistry, who is devoting a large part of his recent efforts to the investigation of the relationships between Chemistry and ethical choices of scientists.

This expression has been the leitmotiv of a series of initiatives carried out in Italy, in Europe and in Asia (2) aiming at enhancing broad public's awareness on the potential risks and threats linked to the *dual use* (for either malicious or peaceful purposes) of chemical know-how and compounds.

Hazardous industrial chemicals, explosives, chemical weapons and polluting industrial materials are well known examples generating fear and increasing the general sensation of vulnerability in non-expert population. Technogenic incidents, either deliberate (terrorist attacks) or unintentional (industrial accidents), are indeed felt as a major source of concern by the public opinion. However, a poor risk assessment when facing emergency situations and/or incidents with hazardous chemicals can induce a sense of impotence and inability in tackling the non-conventional event in expert professionals too, if they are not properly trained and skilled.

In this scenario, only a better knowledge can minimise fear and only adequate awareness-raising actions addressed to wide audiences can enhance people's preparedness and resilience against chemical disasters and threats.

Education, dissemination and training activities organised in schools, universities, governmental agencies and professional bodies are a powerful tool to discredit wrong common places, rectify false myths and, in general, to help people to be more familiar with “good” Chemistry and its concepts.



Figure 1. (from left to right). “Chemistry for Safety and Security” at the 9th Edition of the European Night of the Research, in Alessandria; training courses for governmental first responders in South-East Asia: hand-over of certificates in Lao and table-top exercises with Cambodian delegates.

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From the Marotta's Institute to Sapienza University passing through Camerino: Sixty years spent working in the field of chemistry.

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The occasion of awarding to Professor Domenico Misiti this prestigious medal bearing the name of Domenico Marotta represents a favorable occasion to remind and honor the figure and personality of an open minded chemist who even had the privilege of knowing Marotta personally and gained his friendship and esteem for long time since the beginning of his scientific career in 1956.

The various and different aspects of Misiti's scientific activity will be briefly and schematically reviewed, starting from his researches in the field of medicinal and natural substances chemistry under the guidance of Daniele Bovet and G.B.Marini Bettolo.

His research activity concerned mainly the synthesis of biologically active heterocyclic compounds, structure elucidation of natural compounds, asymmetric synthesis, separation science, synthesis of new chemio- and stereo-selective chiral stationary phases, studies on the mechanisms of stereoselective molecular recognition, development of new analytical methods in the field of biosciences, biotransformations and biocatalysis, chemistry of calixarene and fullerene derivatives as biological models. In parallel to the research and teaching activity and in addition to the numerous institutional assignments, an intensive organizational and dissemination activity has been developed mainly in relation to drugs and to chemical risk to health and the environment in National and International Institutions such as CNR in "Fine Chemistry I°-II° Projects", OCDE, EEC, EMEA, European Pharmacopoeia and MiUR, MSE, Ministry of Health, Ministry of Environment and several National Regions as Expert in the evaluation of numerous industrial research projects. Moreover an industrial consulting position was held mainly for a Pharmaceutical Industry. He promoted also the series of Symposia in Chiral Discrimination (ISCD) and he created the prestigious "Chirality Medal" in Rome in 1991. Finally he also had an editorial activity editing various textbooks for university as well for secondary school students.

D.M would like to thank his Colleagues B. Botta, L. Caglioti, F. Gasparrini, M. Pierini, C. Villani, G. Zappia for their active contribution to his research activity and R. Ballini, S. Cacchi and F. De Angelis for the numerous occasions of scientific interactions with them.

Far comprendere la chimica per fare amare la chimica Elogio della didattica

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La relazione, redatta in occasione del conferimento al sottoscritto della Medaglia Illuminati per la didattica 2017, partendo da un quadro della situazione in cui l'autore si è venuto a trovare nel momento della scelta degli studi universitari, espone le difficoltà incontrate che sono state però di stimolo per il successivo percorso professionale. Consapevole della grande inadeguatezza della scuola frequentata in rapporto alle discipline scientifiche sperimentali, non appena intrapresa la strada dell'insegnamento ha fatto avanzare insieme una sua necessaria autoformazione (in mancanza di qualsiasi sistema di formazione allora esistente nel Paese) e la messa a punto di un percorso didattico innovativo per le scienze sperimentali, in particolare per la chimica, che fosse realmente efficace oltre che sostenibile. Attingendo a tipi di nuovi curricoli che venivano messi a punto in alcuni Paesi anglosassoni (USA e Gran Bretagna) e alle riflessioni sull'esigenza di una nuova didattica sostenuta da vari ricercatori soprattutto europei, l'autore ha messo a punto gli elementi caratterizzanti del proprio nuovo paradigma didattico messo in atto all'interno di una sperimentazione realizzata nella propria scuola. Si è passati cioè da una didattica verbalistica, astratta e tale da rendere l'allievo ascoltatore sostanzialmente passivo di fronte alle spiegazioni del docente, all'adozione di una didattica caratterizzata da alcuni elementi costitutivi che guidano lo studente, a partire da una situazione problematica iniziale opportunamente progettata, alla concreta costruzione dei concetti da acquisire con un confronto generale in classe per una loro condivisione e una conclusiva verbalizzazione del processo effettuato.

Il percorso di insegnamento si è alimentato con una costante attività di ricerca e sperimentazione didattica che nel corso di molti anni ha toccato diversi settori di cui i più significativi sono stati: indagini sull'insegnabilità a determinati livelli scolari di alcuni concetti-chiave della chimica, didattica del laboratorio e rapporti tra teoria ed esperienza, problem solving, verifica e valutazione degli apprendimenti in chimica e controllo delle competenze acquisite. Accanto a queste ricerche e sperimentazioni sono stati sviluppati altri due settori di interesse: da un lato l'esigenza di opportune riflessioni sugli aspetti epistemologici e metodologico-didattici dell'insegnamento della chimica e dall'altro l'esigenza di creare e far funzionare strutture e competenze per una nuova formazione primaria e in servizio dei docenti. Ad un primo livello di organizzazione l'autore si è mosso come membro della Divisione Didattica della SCI di concerto con le altre Associazioni di insegnanti di scienze sperimentali (Fisica, Biologia e Scienze della Terra). La vincita del concorso a Supervisore lo ha poi portato all'interno delle nascenti Scuole di Specializzazione degli Insegnanti di Scuola secondaria (SSIS) a collaborare con colleghi dell'Università di Firenze e a svolgere anche l'incarico del corso di Laboratorio di didattica e didattica del laboratorio. Attualmente fa parte del Comitato scientifico del gruppo di lavoro creato dalla Regione Toscana per la formazione di docenti di discipline scientifiche in servizio "Laboratori del sapere scientifico" (LSS) in funzione da ormai 10 anni e svolge attività di formazione.

Conclude la relazione un appello alla comunità dei chimici sullo stato della ricerca didattica, la necessità di sostenere una nuova formazione primaria dei docenti e infine l'esigenza di omogeneizzare l'insegnamento della chimica a livello di scuola secondaria superiore mediante la creazione di un'abilitazione bidisciplinare, come emerge da un puntuale documento messo punto tre anni fa da una qualificata commissione della Divisione Didattica della SCI e presente sul nostro sito.

Solid state quantum chemistry: towards the rational design of nano- and photo-catalysts

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The rational design of advanced materials is an ambitious target of modern chemical research. Thanks to the advances of quantum theory methods to determine the electronic structure of solids and to describe complex chemical systems and reactions, nowadays not only it is possible to rationalize experimental observations, but also to predict novel systems with potential interest in practical applications. Two fields where progress has been particularly relevant are nanocatalysis and photocatalysis.

Nanocatalysis deals with components of a solid catalysts at the nanoscale. A way to exploit nanodimensionality in heterogeneous catalysis is to use oxide nanostructures. Graphene is the prototype of two-dimensional (2D) materials, but also oxides can be prepared in this form. When 2D oxides are grown on a metal, new physical properties and chemical reactivity appear, opening the way towards new catalytic systems. A relevant example is that of gold nanoclusters on MgO, FeO, and other oxide ultrathin films, and of the spontaneous charging effects that they induce.

Photocatalysis deals with the use of materials able to efficiently transform solar energy into chemical energy. A lot of efforts have been dedicated to this topic in the last decades, with alternating success. Introducing dopants, defects, heterojunctions, etc. opens a great number of possibilities to engineer new semiconducting oxides. This can be efficiently explored with the help of quantum chemistry which can provide new insight, concepts, and ideas.

In this talk we will discuss selected successful examples of nano- and photo-catalysts derived from theoretical models, showing the potential that solid state quantum chemistry has to solve problems in material science in general, and in heterogeneous catalysis in particular.

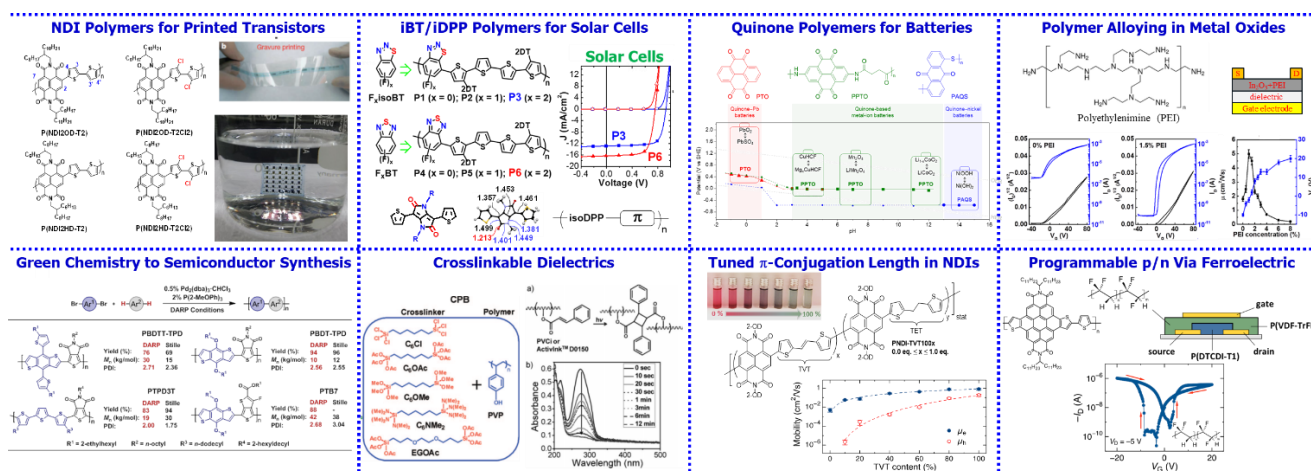
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Polymers and Polymeric Composites for Flexible Opto-Electronic Devices

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In this presentation we will describe the design rationale, synthesis, characterization of several organic semiconducting and dielectric materials for printed/flexible thin-film transistors (TFTs), (1-5) circuits, (4) photovoltaic cells (PVs), (6,7) and batteries (8) as well as to understand their charge-transport/performance characteristics as a function of the device architecture and interface modifications (Fig. 1). Furthermore, new hybrid materials comprising polymers and metal oxide semiconductors will be presented. (9,10) We will also briefly summarize our recent synthetic efforts for the sustainable synthesis of semiconducting polymers. (11,12) Finally, new approaches to understand how the degree of π -conjugation in semiconducting polymers affect charge transport will be reported. (13) Our materials enable the realization of printed TFTs with mobilities $> 3\text{-}40\text{ cm}^2/\text{Vs}$, OPV cell with efficiencies $> 12\%$, and aqueous batteries with specific capacities $> 395\text{ mAh g}^{-1}$.



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Exploring the cytotoxic, apoptotic and antitumoral effects of two new gold N-heterocyclic carbene–gold(I) complexes on A2780 human ovarian cancer cells

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Following the introduction of auranofin in the clinics for the oral treatment of rheumatoid arthritis and the discovery of its remarkable antiproliferative properties *in vitro*, gold compounds were increasingly considered and evaluated as a possible source of new and more effective metal-based anticancer agents (1). This interest was also fueled by the observation that gold compounds usually manifest a very different pharmacological profile compared to established anticancer platinum drugs, implying the occurrence of original and innovative modes of action. Among the various families of gold compounds tested for their anticancer effects in the last decade, a variety of organometallic gold(I) N-heterocyclic carbene (NHC) complexes were designed, featuring anticancer activity in the micromolar or sub-micromolar range *in vitro* (2,3). In this frame, we show here two gold carbene compounds, Au(NHC) and Au(NHC)₂, endowed with potent cytotoxic properties *in vitro* toward various cancer cell lines. We explored the cellular and molecular mechanisms that are at the basis of their antiproliferative properties. Both carbene complexes affected proteins belonging to protein synthesis, metabolism, cytoskeleton and stress response and chaperones. To obtain a more detailed view of these metabolic differences we evaluated the ability of carbenes to affect glycolytic and mitochondrial activity.

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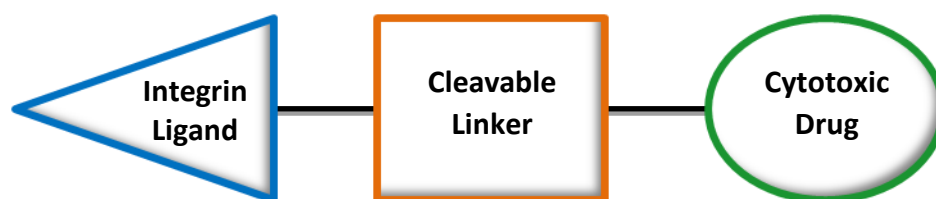
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Tumor Targeting with Integrin Ligand - Drug Conjugates

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Integrins are a large family of heterodimeric transmembrane glycoprotein receptors, composed by two non-covalently-associated subunits (α and β). Integrins $\alpha_v\beta_3$ and $\alpha_v\beta_5$ have been found to be overexpressed on blood vessels in tumors, but not on vessels in normal tissues. For this reason, these integrins have become attractive targets for pharmacological studies mainly in the oncology area. We have recently investigated the synthesis and biological properties of a new class of cyclic peptidomimetics containing a bifunctional diketopiperazine (DKP) scaffold and the tripeptide sequence Arg-Gly-Asp (RGD) (1,2) or *iso*Asp-Gly-Arg (*iso*DGR) (3) as potent integrin ligands. Competitive binding assays for the displacement of biotinylated vitronectin bound to purified $\alpha_v\beta_3$ and $\alpha_v\beta_5$ integrins displayed excellent IC₅₀ values, in the low nanomolar range. The interaction of *cyclo*[DKP-RGD] ligands with intact cancer cells was investigated by NMR and computational studies, allowing the determination of the binding epitope and the bioactive conformation of the ligands (4). *Cyclo*[DKP-RGD] and *cyclo*[DKP-*iso*DGR] ligands proved to be potent angiogenesis inhibitors and genuine integrin antagonists (5). Since α_v integrins are overexpressed on the surface of cancer cells, integrin ligand-Paclitaxel conjugates were synthesized with the aim of using the tumor-homing *cyclo*[DKP-RGD] or *cyclo*[DKP-*iso*DGR] peptidomimetics for site-directed delivery of the cytotoxic drug (6,7,8).



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Can chemistry replace the scalpel? The case of photodynamic therapy

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Photodynamic therapy (PDT) is a non-invasive medical therapy nowadays used for the treatment of different kinds of tumors (e.g. esophagus, bladder, early lung, breast and prostate cancers), age-related macular degeneration, skin diseases and its clinical efficiency is currently explored for other diseases such as infections, cardiovascular and environmental application (e.g. water treatment and disinfection processes). For the origins of phototherapy, the roots can be found in the Egyptian and Greek culture many thousand years ago. In the 1892-3 years Sciascia in Palermo and Finsen in Stockholm demonstrated the possible use of the light in medicine. The therapeutic use of light began in 1900 when Raab reported that the combination of acridine orange and light could destroy living organisms. Nowadays, it is used in oncology and ophthalmology in United States, Japan, Canada, France, Netherlands and other 8 countries. A series of drugs including Levulan (D-5-aminolevulinic acid), photofrin (sodium porphyrin), SnET2 (Sn-ethyl-porphyrin), MV9411 (In), Lutrin (lutetium texaphyrin) and others are commercially available for cancer therapy. PDT requires the combination of a light source of adequate wavelengths with an appropriate photosensitizer. In given physico-chemical conditions, this mix can produce excited singlet molecular oxygen that is the cytotoxic agent. Then, we can define PDT as a “surgery without scalpel” or a surgery with a chemical scalpel (O_2 , $^1\Delta_g$).

In this talk, I will briefly review our works (1) in this filed underlying as theoretical and computational chemistry should be a potent tool in designing and proposing new efficient drugs for photodynamic therapy.

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Towards the Greening of Oxidation Reactions

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Catalytic oxidation is intrinsically a poorly selective reaction because in general the reaction product is more easily oxidizable than the starting substrate, this leading very often to a number of unwanted by-products. Since the early 1980's hydrogen peroxide has been successfully employed as an environmentally acceptable oxidant, replacing a variety of less benign mono-oxygen donors, in a range of synthetically useful organic chemistry reactions such as sulfoxidation, alkene epoxidation, the hydroxylation of aromatics, the Baeyer-Villiger oxidation of ketones (1). These processes were made possible by the use of transition metal catalysts possessing soft Lewis acidity properties thus opening the way to nucleophilic oxidation (2) proving very profitable in terms of selectivity in all its declinations: chemo-, regio-, stereo-, enantio-.

More recently these systems were further improved in terms of sustainability by carrying out the above reactions in water with the aid of self-assembling additives like surfactants, opening the way to other synthetically useful reactions like hydration, hydroformylation, C-C bond formation (3) all characterized by sometimes large selectivity improvements. This practical approach allowed to expand their application potential because not only they represent examples of Green Chemistry, but they can also shorten costs and working times mainly in multi-step processes employed in the pharmaceutical sector as has been recently demonstrated (4).

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Speaker Invitati

Chimica per la tutela dell'ambiente e del patrimonio culturale *Chemistry for environmental protection and for preservation of cultural heritage*

Martin Scheringer	ETH Zürich, Department of Environmental Systems Science
Koen Janssens	University of Antwerp, Campus Groenenborger
Maria Cristina Facchini	CNR, Istituto di Scienze dell'Atmosfera e del Clima (CNR-ISAC)

Etica e Scienza

Enrico Bucci	Resis Srl, Italy; Sbarro Health Research Organization, USA
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Chimica per l'economia circolare - Chemistry for circular economy

Vincenzo Balzani	Alma Mater Studiorum - Università di Bologna, Dipartimento di Chimica "Giacomo Ciamician"
Ryu Abe	Department of Energy and Hydrocarbon Chemistry, Graduate School of Engineering, Kyoto University,
Anders Hagfeldt	Ecole polytechnique fédérale de Lausanne, Institut des sciences et ingénierie chimiques
David Peck	Delft University of Technology, Faculty of Architecture and the Built Environment

Chimica per la salute - Chemistry for health

Paola Arimondo	CNRS - Centre Pierre Fabre Laboratories - Research & Development
Aldo Roda	Università di Bologna, Dipartimento di Chimica "Giacomo Ciamician"
Giuseppe Legname	Scuola Internazionale Superiore di Studi Avanzati - Neurobiology Sector
Christian Amatore	Ecole Normale Supérieure Département de chimie

Produzione sostenibile e sviluppo economico *Sustainable production and economic development*

Vittorio Maglia	Federchimica
Johannes A. Lercher	Technische Universität München, Department Chemie
David Cole Hamilton	School of Chemistry, University of St. Andrews
Oliver Kappe	Kerl-Franzens-Universität Graz, Institut für Chemie
Paul T. Anastas	Department of Chemistry, Yale University
Francesca Ferrazza	Eni S.p.A. - Research & Innovation

Chimica e Sport - Chemistry and Sport

Santo Davide Ferrara	Università di Padova
Luigi Nicolais	Università di Napoli Federico II

Eventi satellite di interesse industriale - Satellite events of industrial interest***Grafene e sue possibili applicazioni industriali***

Gaetano Granozzi	Dipartimento di Scienze Chimiche-Università di Padova
Giovanni Bruno	Istituto di Nanotecnologie-CNR Nanotec Bari
Maurizio Galimberti	Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta"-Politecnico di Milano
Michele Maggini	Dipartimento di Scienze Chimiche-Università di Padova
Zhenyuan Xia	Istituto per la Sintesi Organica e la Fotoreattività -CNR-Bologna
Maurizio Peruzzini	Istituto di Chimica dei Composti Organo Metallici-CNR-Firenze
Manuela Melucci	Istituto per la Sintesi Organica e la Fotoreattività-CNR-Bologna
Maria Rosaria Acocella	Dipartimento di Chimica e Biologia, Università degli Studi di Salerno
Pellegrino Musto	Istituto per i Polimeri, Compositi e Biomateriali -CNR Pozzuoli
Marino Lavorgna	Istituto per i Polimeri, Compositi e Biomateriali-CNR Portici
Michele Giordano	Istituto per i Materiali Compositi e Biomedici-Portici

Formulazioni nell'industria chimica e farmaceutica

Vittorio Maglia	Federchimica
Marco Adami	Pharmaceutical Consultant, Milano
Sesto Viticoli	Italian Association for Industrial Research
Enrico Zambelli	Chiesi Farmaceutici S.p.A.,
Giorgio Ferrari	Mapei S.p.A.,
Salvatore Mercuri	Micro-Macinazione SA
Franco Gasparri	MedaPharma S.p.A.,
Stefano Resta	Fater S.p.A
Antonino Bagnulo	Fater S.p.A
Massimo Bonini	Consorzio per lo Sviluppo dei Sistemi a Grande Interfase (CSGI)
Pasquale Del Gaudio	Università di Salerno
Martino Di Serio	Università di Napoli Federico II

Conferenze Plenarie

Environmental Chemistry: Quo Vadis?

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Environmental chemistry deals with the fate (i.e., the transformation and degradation, phase partitioning, and transport) of anthropogenic chemicals in the environment. This field of research combines original scientific research (elucidation of processes governing the fate of chemicals in all environmental media; development of sampling techniques and measurement methods, etc.) with decision making processes (chemical risk assessment, input to development of chemical policies) at the national and international level, for example for the European chemicals regulation, REACH, and the Stockholm Convention on Persistent Organic Pollutants (POPs), an international agreement. Over the last 50 years, environmental chemistry has made important contributions to the scientific understanding of how chemicals circulate in, and interact with, the environment (1), including the elucidation of the mechanisms leading to stratospheric ozone depletion (Nobel Prize in chemistry in 1995); detection of anthropogenic chemicals in remote areas, including the bottom of the Mariana Trench, snow of the Himalayas, and waters around Antarctica; and development of highly sensitive analytical methods applicable to many different chemicals present and complicated matrices. Another genuine contribution of environmental chemistry is the education of scientists who play a crucial role in industry and governments in the process of chemical risk assessment. Whereas the role and relevance of environmental chemistry (and the related field of ecotoxicology) is clearly recognized in industry and governments, environmental chemistry and ecotoxicology have been losing support, resources and recognition at universities for many years (2). What are possible causes of this process? A first problem may be that the need for research and teaching in environmental chemistry and ecotoxicology is no longer seen at universities because chemical pollution problems are considered as largely solved. Secondly, environmental chemistry and ecotoxicology may be seen as fields dominated by routine work and where there are not many interesting research questions left. A third part of the problem may be that other environmental impacts such as climate change are given higher priority than chemical pollution problems. Here, all three possible causes of the loss of recognition of environmental chemistry are discussed and several cases are presented that illustrate the great demand for innovative research and teaching in environmental chemistry and ecotoxicology. It is crucial that environmental chemistry and ecotoxicology are firmly rooted in academic science and are provided with sufficient equipment, resources and prospects for development (3).

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The chemistry of Pigment Degradation: Investigations at different Length Scales

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Many painting materials employed by artists in different historical periods, ranging from the Antique period to the modern era, are subject to spontaneous degradation [1]. Usually, a combination of physical and chemical factors in the environment of the works of art exert an influence on the durability of the pigments originally employed. This can lead to a loss of mechanical strength of the paint as a whole but can also take milder forms such as a discoloration. Often discoloration phenomena are caused by redox transformation of original pigments. In the recent past, we have examined the degradation of various sulfide-based pigments such as vermilion red (HgS), cadmium yellow (CdS) and orpiment (As₂S₃) used in well-known works of art by Van Eyck, Rubens, Rembrandt, Van Gogh and Munch.

Many of these substances are semi-conductor materials that upon illumination with light of sufficient energy can release electron-hole pairs that in their turn can promote oxidation and reduction reactions, either of the semi-conductor material itself or of materials in its immediate vicinity. In this presentation, the attention will be focussed on the degradation of lead and arsenic based pigments employed by artists and craftsmen in different period. Minium (also known as *red lead*, Pb₃O₄) is a mixed-valence oxide of lead that can be converted to various lead carbonates, hereby losing its characteristic red-orange color [2]. Some forms of chrome yellow, a class of pigments frequently used by artists at the end of the 19th century are prone to photo-reduction while others are much more stable under exposure to light [3]. An unstable class of pigments used in many historical periods are arsenic sulfides (in general As_xS_y) that may first convert into arsenolite (As₂O₃) and upon further oxidation to very mobile arsenate compounds [4].

The degradation pathways of these pigments can be elucidated as a function of environmental conditions by means of a combination of (X-ray based) analytical imaging methods such as X-ray fluorescence, X-ray diffraction and X-ray absorption spectroscopy. Macroscopic forms of these methods [5] are employed to characterize and explore the affected works of art in their totality while microscopic variants are useful for more detailed (speciation) analysis of minute paint samples taken from these artworks [1,2]. A number of case studies will be discussed as concrete illustrations.

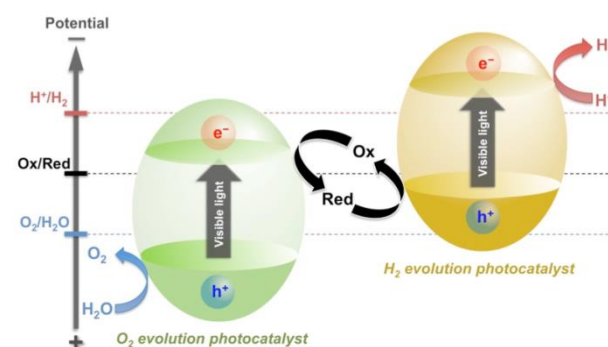
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Mixed-Anion Semiconductor Photocatalysts for Visible Light Induced Water Splitting

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Photocatalytic water splitting into H₂ and O₂ using semiconductor photocatalysts has received much attention recently due to the potential for the clean production of H₂ from water utilizing solar energy (1). Because almost half of all incident solar energy at the Earth's surface falls in the visible region, the efficient utilization of visible light remains indispensable for realizing practical H₂ production. We have recently developed a new type of photocatalytic water splitting system, mimicking the mechanism of photosynthesis in green plants (2). In this system, the water splitting reaction is broken up into two stages: one for H₂ evolution and the other for O₂ evolution; these are combined by using a shuttle redox couple (Red/Ox) in the solution. Over a H₂ evolution photocatalyst, the photoexcited electrons reduce water to H₂ and holes oxidize a reductant (Red) to an oxidant (Ox). The Ox is reduced back to the Red by photoexcited electrons generated over an



O₂ evolution photocatalyst, where the holes oxidize water to O₂. This system reduces the energy required to drive each photocatalysis process, allowing visible light to be utilized more efficiently than in conventional water splitting system. We have achieved overall water splitting using various visible light responsive photocatalysts, such as SrTiO₃ doped with Cr (2), tantalum oxynitrides (TaON or BaTaO₂N) (4), and organic dyes (5), which work as a H₂ evolution photocatalyst, combined with tungsten oxide (WO₃) for O₂ evolution in the presence of a shuttle redox mediator such as iodate/iodide (IO₃⁻/I⁻). We have recently demonstrated that some oxyhalides such as Bi₄NbO₈Cl, with single layer Sillen-Aurivillius perovskite structure, are stable and efficient O₂-evolving photocatalysts under visible light, enabling a Z-scheme overall water splitting with Fe³⁺/Fe²⁺ redox (6). It was revealed that the valence band maximum of Bi₄NbO₈Cl is unusually high owing to highly dispersive O-2*p* orbitals (not Cl-3*p* orbitals), affording the narrow band gap and the stability against self-oxidative deactivation. We have also demonstrated that the porous tantalum oxynitrides (TaON or BaTaO₂N) film electrode prepared on conducting substrates showed stable O₂ evolution with significantly high quantum efficiency in an aqueous solution, after loading of IrO₂ or CoO_x nanoparticles as a cocatalyst for water oxidation; enabling water splitting into H₂ and O₂ under visible light with a Pt electrode under an externally applied bias (7).

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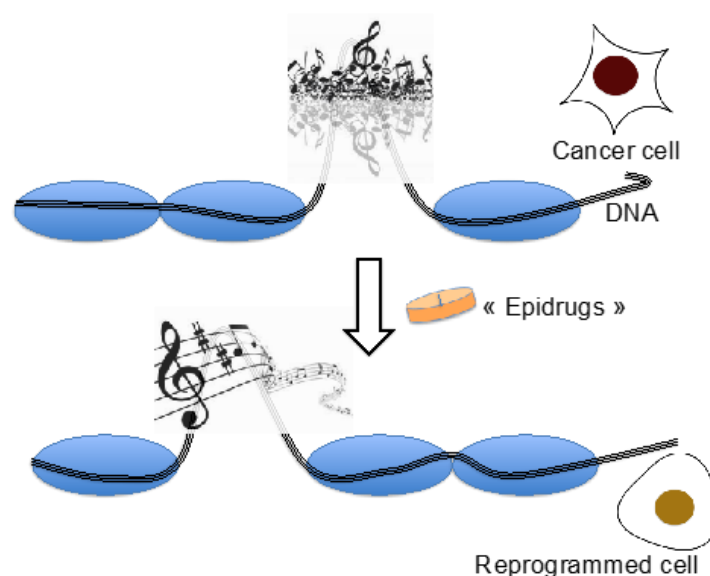
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Towards the reprogramming of cancer cells with chemical tools targeting DNA methylation

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DNA methylation is involved in the regulation of gene expression and plays an important role in normal developmental processes and disease. In particular, the epigenetic landscape is altered in cancers where abnormal hypermethylation leads to silencing of certain genes such as tumor suppressor genes. In mammals, DNA methyltransferases are the enzymes responsible for DNA methylation on the position 5 of cytidine in a CpG context. Few direct enzyme inhibitors are known and those have several drawbacks. In order to identify novel inhibitors, we developed three chemical strategies. First a fluorescent High-Throughput Screening for the inhibition of the murine catalytic Dnmt3a/3L complex. Second, based on molecular modeling studies of quinoline inhibitor SGI1027 and *N*-Phthaloyl-L-tryptophan RG108, we found four compounds induced the reexpression of a reporter gene, controlled by a methylated CMV promoter, in leukemia KG-1 cells. Third, we design bisubstrate analogues of the DNMTs and found potent quinazoline-based compounds active in cancer cells. Finally, docking studies were conducted in order to understand their binding mode. The biological activity of the compounds was also addressed in solid and hematological cancer cells. Altogether, these studies provide insights for the design of the next-generation of DNMT inhibitors.



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Advanced instrumentation for the astronaut health monitoring and diagnostics during long-term space exploration

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Life evolved on Earth, while the force of gravity has been constant for billion years and there is no genetic memory of life responding to gravitational force changes. Space microgravity is therefore an unnatural place to live. But what happens to humans in space? Many physical properties of solids and liquids are different in microgravity, including capillarity, hydrostatic pressure, surface tension, wettability, buoyancy and thermal convection. We therefore expect that this new environment greatly affects the human physiology even at a cellular level, which becomes even more relevant and critical in extended duration missions. The main microgravity negative effects on astronaut's health and performances result from fluids and organs shift-up causing edema and optical nerve distortion and the vision grows worse. Furthermore, without the constant tug of gravity skeleton doesn't work nearly as hard, which causes it to weaken and decalcify.

Additionally to microgravity, the major biological risks of space travel derive from cosmic rays, loss of atmosphere, exposure to toxins, mechanical trauma, acceleration and deceleration, extreme temperatures, meteoroids and space debris, circadian rhythms and sleep alterations and psychological distress. The safety and success of extended space missions require efficient management of astronauts' health by monitoring a range of physiological parameters that are indicators of the health status and by setting up a real autonomous clinical care in the space station. The chemistry of smart materials and nanostructures is a key point, not only for the spacecraft structure, but for health: radiation shielding using quantum dots, for example, which can tolerate hundreds of times more radiation than their macroscale counterparts can; isotopically-enriched boron nanotubes might be able to effectively shield radiation and store energy as they form the hull of a spacecraft. Nanotechnology makes "lab-on-a-chip" solutions with instant results possible, thus boosting biosensor applications, which are crucial to space exploration for monitoring astronaut health and water quality, and for seeking out life on other planets. The medical equipment toward and independent clinical care should perform diagnostics tests, body imaging (ultrasound, X ray) and even surgery in case of emergency by a non-medical personal. The use of tele-robotic and telemedicine will allow approaching part of these problems.

The main avenues using nanotechnology and nanomaterials for scaling down a gravitational independence diagnostic system's footprint are: 1) reduce the scale at which the device operates at nanoliter volume levels. 2) Include on board biosensors based on optical and electrochemical detection which are nowadays mature, driven by micropumps and valving integrated with electronics to achieve the needed robustness and ruggedness. 3) Exploit shared resources such as PC, CCD for data analysis and processing. 4) Scale back the disposables. 5) Incorporate modularity via dynamic programmability by using quick disconnects or swiping out chip. 6) Use a device that can perform massive multiplexing, i.e. process many tests from a single sample with high sensitivity and non-invasiveness.

Our experience in space medicine diagnostics, dealing with the development of portable devices and biosensors to non-invasively measure health biomarkers in astronauts' breath and saliva, respectively from MARS 500 Mars simulation mission and on board International Space station ISS experiments, will be reported and discussed, as examples of the role of chemistry in space medicine. The most appropriate methodological approaches in term of analytical principle, format, instrumentation will be critically discussed, anticipating the new advanced emerging technology.

**Lessons from enzymes -
On the role of steric constraints and chemical environments for catalysis**

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Elementary organic transformations are catalyzed by enzymes at large unmatched rate and selectivity. The local constraints at active sites of enzymes and the local chemical environment are two key properties to achieve such extraordinary catalytic vectors. We use the sites in crystalline nanoporous materials to mimic such well-defined reaction space. Molecules experience constraints that can be subtly adjusted via direct synthesis, as well as via the addition of cations, oxidic clusters or organic fragments. The role of water and other solvents in such environments changes drastically the reaction pathways compared with the catalytic pathways in a homogeneous environment of chemistry in solution. The lecture will compare reactions such as elimination reactions of alcohols, alkylation of aromatic molecules and the role of acid sites for hydrogenation and hydrogenolysis. Experimental methods to define the state of the reacting molecules combined with detailed kinetic analysis and theory will be used to explain the principal contributions of the interactions and the confinement to determine reaction rates. It will be discussed how reaction rates and pathways can be tailored using the space available for a transition state and the chemical constituents around the active site.

The catalytic production of chemicals from waste bio-oils

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As oil supplies dwindle and the price increases, it is essential to find new ways of making the many chemicals on which the quality of our lives depends. One possible solution is to use waste products for the manufacture of chemicals. We shall discuss the conversion of fatty acids from *Tall Oil*, a waste from wood processing, into polymer precursors. We shall also discuss the synthesis of a range of important chemicals from cashew nut shell liquid (CNSL), a waste from cashew nut processing.

We shall show how homogeneous carbonylation,(1, 2) metathesis,(3) and reductive amination(4) can be used to make difunctional esters acids, alcohols and amines(1, 5, 6) for polymer formation(7, 8) from unpurified natural oils containing oleate residues. We shall also describe a direct route to *N*-heterocycles from diacid esters and amines.

Cashew nut shell liquid contains interesting phenols *meta* substituted with an unsaturated C₁₅ chain. We shall describe how it can be used to synthesise tsetse fly attractants, potentially safe detergents, polymer additives, monomers for polymerisation and large ring macrocyclic lactones.(9-13) (Figure 1).

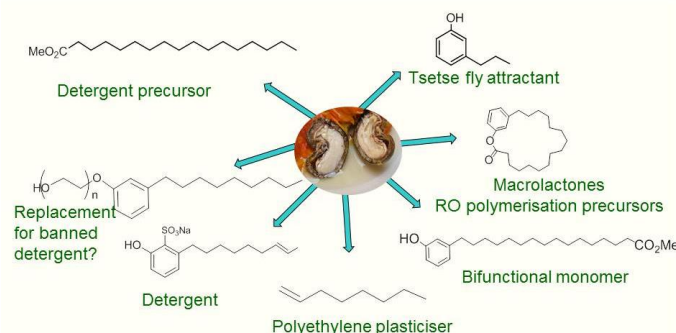


Fig. 1 Chemicals from cashew nut shell liquid

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Keynote e Conferenze su Invito

From a Linear to a Circular Economy The Role of Energy

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Thanks to science, technology and fossil fuel energy, in the last 50 years there has been an increasing human activity that has caused enormous changes in the Earth's system. We are living in the so-called linear economy, an economic model based on the assumptions that resources are infinite and infinite is also the space for disposing waste. The linear economy, which is powered by a non-renewable and dangerous energy source like fossil fuels, causes an irreversible degradation of the planet.

We need to get out of the linear economy and adopt a circular economic model where raw materials are used in the smallest possible quantity and with the highest efficiency to fabricate things designed not only for use, but also for being repaired, reused, collected, and recycled to provide new useful materials. To run a circular economy we need renewable energies that can be obtained from sun, wind, water.

Renewable energies are abundant and, in principle, fossil fuels could be completely replaced by 2050. In practice, however, there are problems because renewable energies must be converted into the forms of energy that we need in everyday life: electricity, heat and fuels. Such a conversion is performed by devices (e.g., PV cells and wind turbines) that must be constructed starting from the elements of the Periodic Table. While some elements are abundant, others are scarce. So the bottleneck for energy production is not the number of photons arriving from the sun or the availability of wind, but the accessibility of the elements needed for constructing devices for energy conversion and storage. Chemistry can play a fundamental role in solving this problem, by: (i) replacing critical elements with other more abundant; (ii) redesigning chemical processes; (iii) reducing the amount of materials used; (iv) increasing efficiency of devices for energy conversion and storage; (v) improving recycling processes.

Energy availability is a very important factor to reach a good level of human development, but above a certain amount of energy consumption any further increase has no effect or it is even damaging. In developed countries there is a need of reducing energy consumption. In principle, this result can be reached by increasing efficiency. Experience shows, however, that increasing efficiency most often does not reduce energy consumption (rebound effects). Effective reduction of energy consumption can only be obtained by focusing on sufficiency, which means reducing use of products or devices.

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The Versatility of Mesoscopic Solar Cells

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In our work on solid-state dye-sensitized solar cells (ssDSSC) we have recently [1] shown that copper phenanthroline complexes can act as an efficient hole transporting material. We prepared ssDSCs with the organic dye LEG4 and copper(I/II)-phenanthroline as redox system and achieved power conversion efficiencies of more than 11%. Our follow up work on electron transfer studies and device optimization will be presented at the meeting.

In our work on perovskite solar cells (PSC) we have achieved efficiencies above 20% with a mixed composition of iodide/bromide and methyl ammonium/formamidinium [2]. For cells larger than 1 cm² we recently certified a record efficiency of 19.6% [3], replacing the anti-solvent step in the perovskite film formation with a vacuum flash treatment. With the use of SnO₂ compact underlayers as electron acceptor contacts we have constructed planar perovskite solar cells with a hysteresis free efficiency above 20% [4]. Recently, we have taken the cation mixing of the perovskite film further by including the Cs⁺ in a so-called 'triple cation' composition, i.e. Cs/FA/Ma. Larger grains grown in a monolithic manner are observed and for example reproducibility and device stability are improved [5]. At the meeting we will discuss our follow up works [6] and present our champion data; up to 22% efficiency with an external electroluminescence of 4%, and an outstanding open-circuit voltage of 1.24 V at a band gap of 1.63 eV entailing one of the smallest loss-in-potential of 0.39 V ever measured for any solar cell material. Furthermore, we will report a breakthrough in stability at 85 °C for 500 h under full solar illumination and maximum power point tracking (during which 95% of the initial performance was retained).

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Critical materials and the circular economy European actions and opportunities

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Rarely in history do we get the opportunity to rethink the entire economic system. The “take-make-waste” way of doing things is coming to an end and Europe is leading the change. Everyone has a role to play in the circular economy which is emerging. In this new world we will reuse, repair, refurbish, remanufacture and recycle products and in doing so value will be created for the benefit of everyone. In the circular economy materials which used to be regarded as ‘waste’ can be turned into the things we all need. It is this significant change that this presentation will cover

Leading universities, businesses, and governments, are currently exploring how to make the circular economy happen. This lecture will give an introduction on what is currently happening and in particular will highlight the problem of critical materials. The opportunities and barriers in the transition towards a more circular system will be explored, and funded programmes and case studies will be shown.

Of Prions and Other Tales

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Prions are unique protein molecules able to replicate in mammal hosts leading to devastating diseases known as prion diseases.

The molecular mechanism underlying prion protein conversion to the infectious form of prion is still quite obscure. Many studies have focused on the structure of the physiological molecule and/or the identity of the pathological form. While the structure of the former is well established, information about the latter is just emerging. In this lecture, I will focus on our knowledge (and mainly our ignorance) about the structural events leading to the formation of a nascent prion molecule.

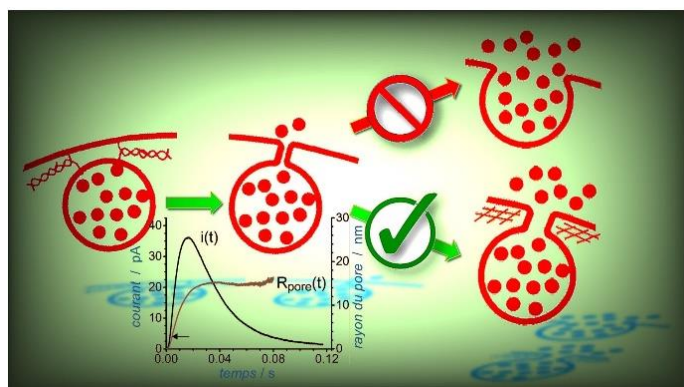
In addition, the relevance of prion conversion and replication mechanisms will be discussed for other proteins involved in neurodegenerative diseases.

Seeing, Measuring and Understanding Vesicular Exocytosis of Neurotransmitters with Micro- and Nanoelectrodes

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Vesicular exocytosis is a biological nanoscale process of crucial importance for cells and tissues communication in humans as well as in most animals. This involves a connection between nanometric vesicles contained inside a cell with the cell membrane occurring by creation of a fusion nanopore across the two membranes through which biologically active molecules stored inside the vesicle are released into the extracellular environment (synaptic cleft, circulating fluids, *etc.*). Despite the minute released amounts (from thousands or millions of molecules), single exocytotic events can be studied by means of the ‘artificial synapse’ amperometric method (1), in which a cell is interrogated by a carbon fiber microelectrode collecting and oxidizing released molecules so that



the finely-structured electrochemical current measured with micro- and nanoelectrodes quantitatively tracks the exocytotic flux. Our purpose in this lecture is to show and explain how this information can be used to derive dynamic information about these phenomena to obtain the time-dependent radius of the fusion nanopore (2). However, the feasibility of such reconstruction requires that one of the characteristic dimensions is known as an independent entry. To this end, we resorted to initial

fusion nanopore radius values (*viz.*, 1.2 ± 0.35 nm), which are well established by patch-clamp measurements. This allowed determining the average neurotransmitter diffusion rate within the vesicle, which in turn permitted reconstructing the fusion nanopore dynamics during neurotransmitter release in endocrine cells (3,4,5). The same approach was used to investigate neurotransmitter release from single functional neuronal synapses, using nanoelectrodes sufficiently small to be inserted inside neuro-muscular synapses (6,7,8).

Owing to the large number of spikes available in amperometric traces this afforded statistically significant distributions of initial and final fusion pore sizes (5,6,7,8). This established unambiguously for the first time that the “full fusion” stage does not end into full fusion but stops after less than ca. 1% of the vesicle membrane surface area is integrated in that of the cell. These results indicate that the fusion mechanism is more complex than thought up to now and is most certainly regulated by an active participation of the actin cytoskeleton or of proteins complexes.

This is an essential finding that rules out a classical paradigm of neurobiology (5,9,10) and may stimulate new medical approaches to treat neurological disorders.

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Organic Synthesis Goes Flow - The Use of Continuous Flow Technology for the Synthesis of Active Pharmaceutical Ingredients

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Continuous flow processes form the basis of the petrochemical and bulk chemicals industry where strong competition, stringent environmental and safety regulations, and low profit margins drive the need for highly performing, cost effective, safe and atom efficient chemical operations. In contrast to the commodity chemical industry, however, the fine chemical industry primarily relies on its existing infrastructure of multipurpose batch or semi-batch reactors. Fine chemicals, such as drug substances and active pharmaceutical ingredients (APIs), are generally considerably more complex than commodity chemicals and usually require numerous, widely diverse reaction steps for their synthesis. These requirements generally make versatile and reconfigurable multipurpose batch reactors the technology of choice for their preparation. However, the advantages of continuous flow processing are increasingly being appreciated also by the pharmaceutical industry and, thus, a growing number of scientists, from research chemists in academia to process chemists and chemical engineers in pharmaceutical companies, are now starting to employ continuous flow technologies on a more routine basis (1).

In this lecture, contributions from our research group in the field of continuous flow processing will be highlighted. Emphasis will be given to highly atom efficient and process intensified chemical transformations useful for the synthesis of APIs or key intermediates that are often too hazardous to be executed in a batch reactor. These involve azide (2), diazomethane (3) and nitration (4) chemistry, selective precious metal-free olefin (5) and nitrogroup (6) reductions, oxidation reactions involving pure oxygen (7) and flow photochemistry applications (8).

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How will Green Chemistry Influence the Future?

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The future will look like largely what we design it to look like. We have spent the past 200 years as a society inventing new technologies that have focused on a very narrow definition of performance and function. While we have revolutionized everything from energy to agriculture to materials, we have also inflicted tremendous harm on the planet and its occupants during the same time period. Green Chemistry supplied the tools and frameworks to allow for designing for sustainability such that new advances can be made while making positive impact for humans and the environment. This talk will focus on the future and the role green chemistry must play.

Marine organic aerosol in Marine Boundary Layer

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Studies performed during the past years suggest that biogenic organic compounds play an important role in submicron marine aerosol chemical composition over biologically productive, high latitude, marine regions, in both hemispheres and new biogenic oceanic sources of primary and secondary origin of OA were revealed. We discuss on the global importance of biogenic OA marine sources, their high spatial and temporal variability and the complex interaction with gaseous biogenic precursors and oceanic biotic components (phytoplankton, viruses and bacteria). Submicron marine organic aerosol are a complex mixture of biogenic materials transferred from the ocean surface by the sea spray or by oxidative gas to particle conversion of volatile organics emitted by decomposition processes of oceanic dissolved organic carbon. The role of marine biota on the evolution of plankton bloom and on the partitioning of oceanic organic carbon in POC and DOC reservoirs and transfer mechanisms into MBL will be presented.

Lies, damned lies: detecting forgeries and manipulations in published scientific images

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Since the commercial introduction of digital imaging software in the '80s, the preparation of high quality images for publication in scientific papers became virtually unlimited. Image production and enhancement, including contrast, luminance and more complex filtering operations, greatly enhanced the clarity of published images, without the need to involve highly skilled artists as it used to be in the past. While this process enhanced the way results are communicated to the public, it also allows several possible forms of misconduct, which range from different types of data falsification to full fabrication of experimental images from scratch. Luckily at the very same time the digitalization of scientific publishing and the emergence of Internet as the main dissemination medium of papers led to the development of tools apt to look for tale-telling signatures in images, so to flag potential manipulations. Some of these tools and the results obtained by large-scale screening experiments will be presented; a general scheme for a standard definition of image manipulation misconduct will eventually be discussed.

Overview of the R&D program at Eni

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In the context of the worldwide growth of the demand for low carbon energy supply, renewable resources will represent an increasingly important part of the energy mix. Nowadays this sector is expanding, particularly in areas where incentives are granted by local and national institutions, with the expectation of developing self-sustaining technologies from the economic, environmental and social aspects. Eni has a broad research and development program focused mainly but not solely on solar energy and advanced biofuels, with the objective of developing clean, sustainable sources of energy for the future energy mix.

Concentrating solar power (CSP) is the oldest and conceptually simplest solar energy technology. The solar radiation is concentrated using lenses or mirrors on a high thermal capacity fluid, heating it to high temperatures for the production of steam. CSP can be integrated in natural gas fueled power stations, and can be equipped with thermal storage to increase its flexibility in steam applications. It is estimated (Roadmap IEA 2010) that CSP will produce 5% of electricity by 2020 in the more favorable areas (12% by 2050 on a worldwide scale). Eni research focuses on the development of advanced parabolic collector prototypes developed in collaboration with MIT and the PoliMi, the identification of innovative low-cost heat-carrying fluids and the development of advanced coatings for receiving pipes, while evaluating the potential for integration with O&G operations.

Organic solar cells (OPV) are a class of emerging photovoltaic devices with interesting potential because they use non-toxic and abundant materials and can be produced using low-cost roll to roll printing technology. The devices currently have lower performances than commercially available modules, in terms of efficiency and lifetime, although steadily progressing thanks to research and development efforts. Eni program on OPV includes the development of innovative patented materials for device fabrication, and of a specific know-how for the fabrication of full modules.

Luminescent solar concentrators (LSC) are made up of sheets of transparent material, either plastic or glass, doped with fluorescent dyes which absorb a part of the sun radiation, re-emitting it a greater wavelength. The light is guided by internal reflection towards the thin edges of the sheet, where it is concentrated on small-sized conventional photovoltaic cells. The performance of this device is closely related to the properties of the fluorescent dyes used. Unlike most traditional photovoltaic modules, these systems also work well at low intensity and non-direct light, thanks to the fact that the dyes are able to absorb sunlight from every direction. Eni has developed patented LSC dyes of various colors, and built a solid proprietary know-how for the realization of working prototypes and demo systems.

Eni's research in the field of advanced bio-oils for transformation in green diesel is engaged in the conversion of **cellulosic waste into microbial oils** with very similar characteristics to vegetable oils. The process uses oleaginous microorganisms (yeasts) able to accumulate a large quantity of lipids inside the cells, which can be extracted and transformed in biofuel for example through the Eni-UOP Ecofining process. The Green Diesel produced in this way can easily be blended with traditional diesel and is completely compatible with present day engines.

Waste-to-Fuel technology thermally converts solid organic waste into bio-oil that can be used for producing electricity or upgraded to diesel fuel. The process is based on a liquefaction process thanks to the water contained in the original biomass. This technology uses raw materials for which an established collection system already exists, and offers an alternative solution to the problem of dealing with waste/sewage sludge from urban areas while respecting the environment.

Sessione del Gruppo Senior: *Chimica e Sport*

Doping-Antidoping and the Role of the Bio-medicolegal Sciences

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The idea that a substance, a product, a magic potion, or a practice can somehow relieve the fatigue and suffering of human life has always been part of cultures in general and perhaps concerns the collective unconscious. Healing and survival have always been transformed in sport into the need to excel and win, even through the use of "potions", "practices" or "doping", experienced without negative values, and applied with shifting strategies, adapted to the evolution of available products, to become "systematic care" that accompanies the athlete throughout their competitive life.

Anti-doping, so far a simulacrum of opposition to the complex and exponential "socio-cultural and sporting" inevitability of the doping phenomenon, has only found positive indications in the recent and rapid evolution of science in the "post-modern society of risk", at once globalized and glocalized. The development of scientific research and the reduction of "black biomedical holes" will benefit from the platforms of the future constituted by imaging, omics and bio-analytical sciences. *Imaging* will evolve at the same pace both in the field of the living and that of the dead, and in the *omics* and *bio-analytical sciences* as well as the clinical and forensic fields.

In the current state of omic maturity, recent innovations in the development of mass spectrometry, cutting-edge technology and computational tools, have considerably increased the power and the potential application of the multi-omic approach, and in spite of the still ongoing progress in the methodologies, their application can already provide informative results leading to more accurate interpretations and evidence.

The integration of omic strategies in the bioanalytical research pipeline has created new opportunities for better understanding the molecular mechanism involved in physiological and pathophysiological states. The methodology has been successfully applied in numerous areas (cancer, cardiovascular disease, obesity, etc.), creating the *Integrative Personal Omics Profile*. Because of its capability to detect slight changes in large datasets, *metabolomics* is also impacting the field of medico-legal disciplines, particularly toxicology, to determine signatures of exposition, susceptibility or toxicity and identify new direct or indirect biomarkers of doping or drug abuse.

Quantitative *Imaging techniques* such as functional MRI, molecular imaging, photoacoustic tomography/endoscopy or the integration of the two, as well as x-ray CT fluorescence molecular tomography, will be the second key platforms of biomedical research in the future. Ptychographic-CT, Optical Frequency Domain, Spectral Optical Tomography and Fluorescence Molecular Tomography will enable the development of algorithms, for the time being based on population data which, if adopted uniformly and applied methodically by the international scientific community, will be able to increase the accuracy of the single discipline.

In the current post-modern society, where Holistic – Personalized and Humanistic Biomedicine is axiomatic, the Evidence can be revealed and understood in full as *Accuracy*, namely, *Truth* equivalent to *Reality*. Moreover, the growing need for certainty in the realm of justice is reflected in the demand for biomedical-molecular, as opposed to opinion-based, evidence.

To be effective and entirely suited to the needs and requirements of the Judicial System, *the future should therefore be* oriented towards the elaboration of a *Mathematical Algorithm* of Evidence, founded on the increased accuracy of the various disciplines. In the meantime, it will be the task of the scientific community and, markedly, of the International Scientific Societies, to sustain an effort of collaboration in the realization of a *Master Plan* on Evidence and Accuracy, so as to be able to definitively declare to the *Justice System* the real capacity of the sciences to furnish truth and proof in doping-antidoping system cases.

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The great changes in the 4th industrial revolution

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The application of Information and Communication Technologies to business processes, the more and more automated and interconnected production processes, and the advent of Internet of Things have anticipated the fourth industrial revolution from which derives the term industry 4.0.

Industry 4.0 is “the comprehensive transformation of the whole sphere of industrial production through the merging of digital technology and the internet with conventional industry” (*Angela Merkel, German Chancellor - Organization for Economic Co-operation and Development, 19 February 2014*).

The fourth industrial revolution is a technological and social change. In fact, the new technologies (I.o.T., cloud, additive manufacturing, big data, advanced robotics and smart materials) often re-structures socio-cultural, political and economic conditions, which in turn change the employment landscape. For example, these technologies (connectivity, computing power, and automation) have given rise to new business models: customer centricity, circular economy, sharing economy, market strategies ICT-based and maker economy.

Grafene e Sue Possibili Applicazioni Industriali

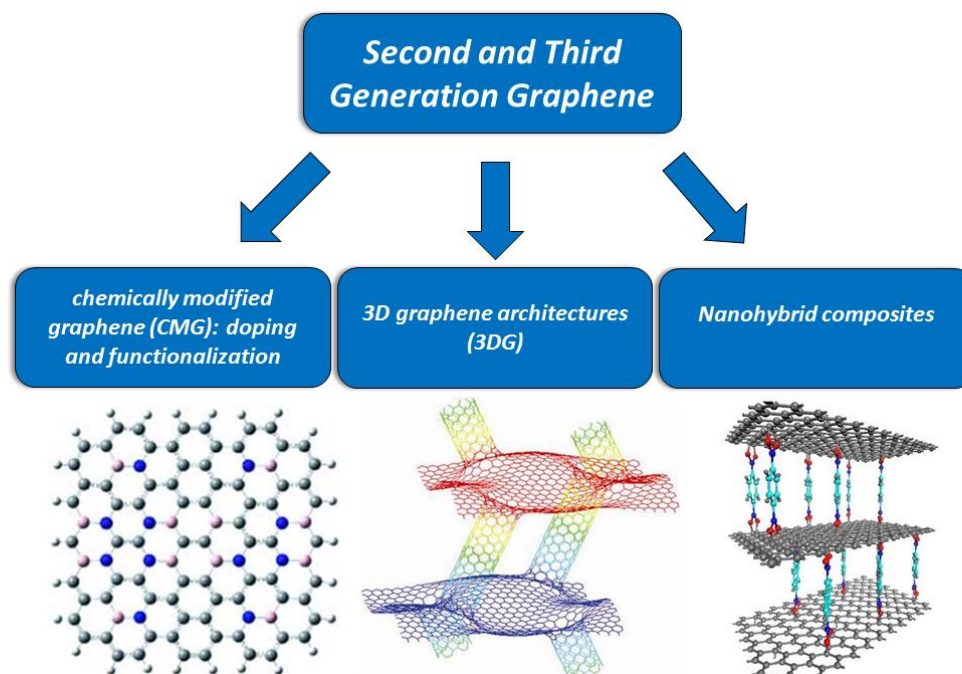
Graphene and Its Possible Industrial Applications

Second and third generation graphenes for energy conversion

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Graphene (G) is an extremely intriguing material that is arousing a formidable interest in many different fields since it was first produced in a conscious manner in a lab in 2003. So many words have already been spent to emphasize its peculiar properties that it is needless to add more efforts to convince scientists on the actual breakthroughs that graphene can provide. Nowadays, the forefront of G research has progressed from the simple preparation and characterization of G toward second generation G-based materials, i.e. chemically-modified graphene (CMGs), and third generation 3D systems based on the assembly CMG sheets (3DGs) or nanohybrid composites with other nanostructures (e.g. nanoparticles or molecules).



The potential of such materials in the field of sustainable energetics (photovoltaics, fuel cells, batteries, supercaps...) has been clearly outlined in recent review articles (1-3). In the present communication the author will briefly summarize the state of the art and will present some recent results from the SSCG of the University of Padova in the field of electrochemical conversion (4-5).

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CVD graphene: transparency, conductivity and flexibility, three inseparable properties to develop innovative applications

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Over the last decade, there has been an intense activity aimed at the development of a synthetic technique capable of producing the “best” graphene, i.e., a graphene that “*clearly reveals itself in a pronounced ambipolar electric field effect*” (1). Nowadays, the most widely used production methods, depending on the specific applications, are the CVD for the growth of large-area graphene films and the graphite exfoliation for the production of large quantities of graphene flakes. However, there is no doubt that the success of the “wonder” graphene is due to three inseparable physical properties that can be considered “graphene values”: transparency, conductivity and flexibility. There have been many efforts to utilize these outstanding properties of graphene in existing and “new” devices for a variety of applications, such as transparent conducting layers in optoelectronics (OLED, photodetectors, photovoltaic cells, touch panel displays,...) (2-7). Although there are many applications demonstrated at lab scale, the development of “best-graphene” technologies is slower than the graphene community expected. The reasons are many and varied, but we have to agree that demonstrating even more the potentialities of the “best graphene” is of primary concern.

The talk will touch on topics that are explored in our lab: CVD graphene growth and transfer on substrates, graphene doping and functionalization. Also, I will share my thoughts on some aspects that require a greater insight into the research for the definitive affirmation of CVD-graphene technology

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Facile and sustainable functionalization method for preparing graphene layers with different solubility parameters

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Graphene has exceptional properties: high charge-carrier mobilities, in-plane thermal conductivity, very high elastic modulus. Such properties essentially arise from the six atoms aromatic ring repeating unit of graphene layers. Hence, objective of graphene synthesis and functionalization should be to obtain and preserve such structure. Graphene functionalization has indeed great importance: electronic and solubility properties, self-assembly and phaseforming behaviour are affected by functional groups.

In this work, a functionalization method was developed (1,2), able to introduce functional groups in peripheral positions of graphene layers, without appreciably altering graphene structure. Functionalization was performed by using molecules whose basic structure is shown in Figure 1. A pyrrole ring with different substituents on the nitrogen atom was used.

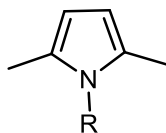


Figure 1

Synthesis of these molecules was performed with high atom economy (larger than 80%), high yield (up to 99%) and thus high atom efficiency, the only byproduct being water, in the absence of solvent and catalyst (3).

Reaction between such molecules and nanosized high surface area graphites was performed by simply mixing them, donating either mechanical or thermal energy. Functionalization occurred with almost quantitative yield. This process has a low environmental impact.

Thanks to such functionalization method, solubility parameter of graphene layer was changed in a broad range, obtaining stable layers' suspension in water, hexane, toluene. From such suspensions, few layers graphenes were isolated. Moreover, even dispersions of graphene layers were prepared in polymer matrices such as poly(1,4-*cis*-isoprene), poly(styrene-co-butadiene), poly(urethane).

This work presents a facile, sustainable, economically viable functionalization method of graphene layers, suitable for preparing few layers graphene from nanosized graphite and for matching the solubility parameters of polymer matrices, achieving even dispersions and intimate interactions.

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Continuous flow synthesis of functionalized graphene

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Microfluidics is a powerful tool for the smart management of chemical reactions. It has been shown that the flow chemistry approach allows for precise control over process parameters, ease of optimization and simplified scale-up from lab-scale to production modules. These features are useful when dealing with complex systems, where reactants are not molecular in nature, as in the case of carbon nanostructures whose chemical functionalization gives nano-sized functional components for a wide range of applications. We focused on the addition to graphene materials of aryl radicals, generated in situ by treatment of aryl amines with alkyl nitrites. This approach has been widely employed for the functionalization of carbon nanostructures. It has been observed that the addition of aryl radicals can result in different layers of the functional molecules being added, therefore a control of both formation and density of oligomers on the graphene surface is needed to prepare derivatives with tailored properties. With this long-term goal, the presentation will outline our results on the covalent linking of different organic molecular structures on graphene and our chemical approach for its non-symmetrical functionalization.

Functionalization and applications of graphene-based materials

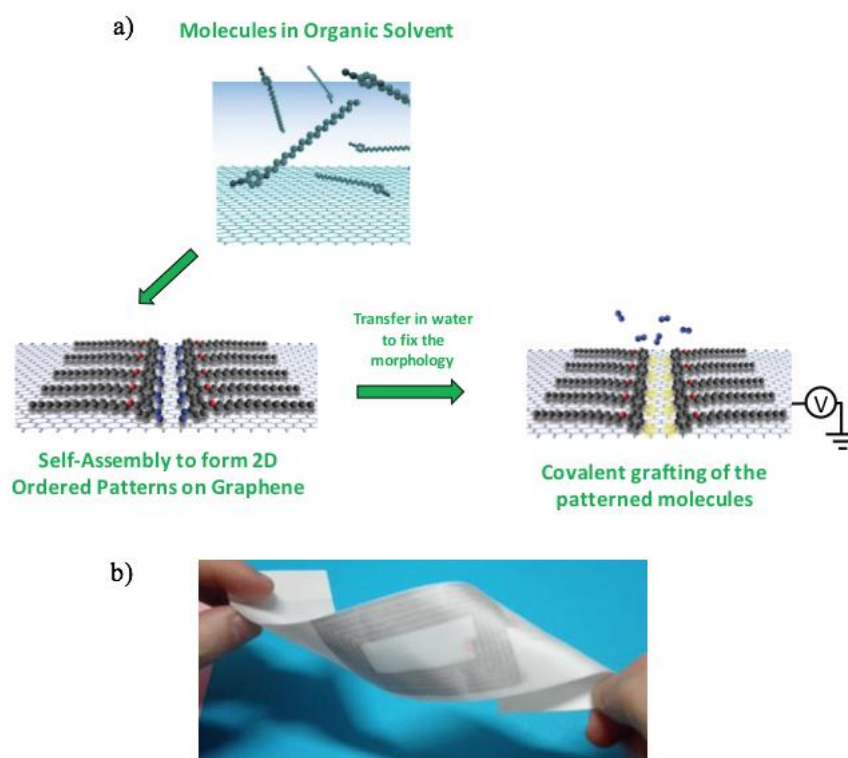
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In this talk, we present some recent results obtained in our group on the chemical functionalization of graphene and a new application of graphene-based materials in flexible electronics.

In particular, we describe a fast and versatile method to functionalize high-quality graphene with organic molecules by exploiting the synergistic effect of supramolecular and covalent chemistry. The approach used is characterized by the independent control over the processes of immobilization of molecules on the substrate and their covalent tethering, enabling fast covalent functionalization of graphene (1).

Moreover, we present a highly flexible Near-Field Communication (NFC) antenna composed of layered materials obtained from re-stacking of graphene nanoplatelets. By combining material characterization, computer modelling and engineering of the device, the antenna could exchange information with NFC readers, such as a mobile phone, matching the performance of standard, commercial metallic antennas. The antennas are chemically inert, highly resistant to thousands of bending cycles and can be deposited on different standard polymeric substrates or silk tissues (2).



a) Scheme of the procedure used for chemical functionalization of graphene. b) Picture of a wearable NFC bracelet in silk with a graphene-based antenna.

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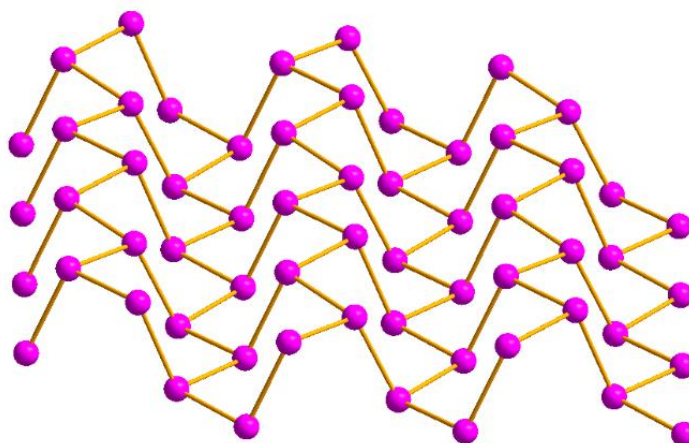
Black Phosphorus: from Ugly Duckling to Black Swan

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Black phosphorus was first synthesized more than one hundred years ago, but until recently it was considered only a scientific curiosity. In 2014 everything changed after the isolation of a new 2D material, the phosphorene, by both mechanical and wet exfoliation of black phosphorus. [1] Just as an example of the huge interest of the scientific community for black phosphorus is the number of papers that was grown exponentially from less than 10 in 2013 to more than 500 in 2016.

Phosphorene is a semiconductor and the value of its direct band gap depends on number of layers between 0.8 to 2.0 eV. This characteristic makes the material very attracting for a large number of applications in optoelectronics such as detectors for near and mid infrared radiation, light-emitting diodes or laser. Also several proofs of concept demonstrated the possibility of building black P-based detectors, modulators, RF transistors, sensors, etc. [2]



On the other side, the material is still in his infancy. Several issues have to be resolved before its full exploitation. In particular, with the aim of wide the material properties as well as to improve its stability and processability in air, we are working in optimizing protocols of reproducible and with high yield synthesis using the wet exfoliation route, the intercalation in different polymeric materials, the construction of devices and the chemical functionalization of this intriguing material. [3-5].

Acknowledgements: The authors thank the European Research Council for funding the project PHOSFUN “Phosphorene functionalization: a new platform for advanced multifunctional materials” (Grant Agreement No. 670173) through an ERC Advanced Grant to MP.

Thanks are expressed to all my colleagues participating in the PHOSFUN ERC project whose names are listed in refs 3 - 5

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Tailored polysulfone-graphene oxide adsorbers for water remediation

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Growing worldwide attention has been paid to the increased occurrence of a vast array of organic contaminants of emerging concerns (EOCs) in urban wastewater system (1). Most of these compounds are recalcitrant to conventional wastewater treatments; consequently they are able to enter ground and even drinking water calling for new treatment technologies. Due to its high surface area, interactions capability with organic molecules and to surface chemical modification possibility, graphene oxide (GO) and GO-based materials are attracting increasing interest for environmental applications (2). In this presentation we summarize our work on the design, tailoring and synthesis of new GO based composites to be used as adsorbers of organic contaminants from water. In particular the synergy of GO and polysulfone (PS), an hydrophobic polymer widely exploited for the fabrication of ultrafiltration membranes, for the removal of seven selected EOCs including pharmaceuticals and personal healthcare products is highlighted. Starting from tailored mixtures of PS and GO (5% w/w) we exploited phase inversion method to fabricate nano/microporous PS-GO composite adsorbers (Fig. 1) that were able to remove ofloxacin (antibiotic), benzophenone-3 (UV filter), rhodamine b (xanthenic dye), diclofenac (antiflammatory) and triton X-100 (surfactant) with efficiency higher than 90% with capacity in the range of tens of mg per g of adsorber, in a few hours treatment times (1-4 h). The mechanism of adsorption in relation to the molecular structure of the organic contaminant was rationalized in terms of hydrophobicity and dipole moment. PS-GO membrane adsorbers outperformed a commercial granular activated carbon (GAC) at low contact times and compared well at longer contact time for the majority of the targeted contaminants, suggesting the suitability of PS-GO composites for advanced water treatment.

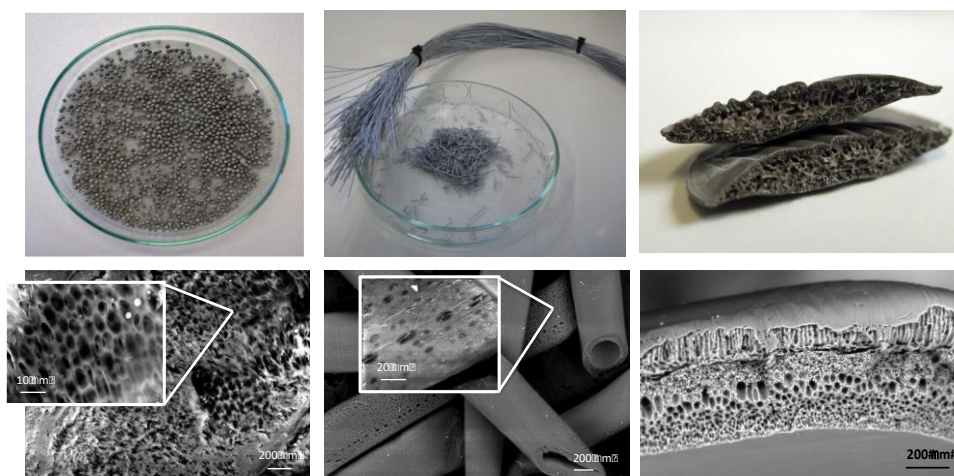


Fig. 1. PS-GO porous composites (top) and morphologies (scanning electron microscopy images).

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New Applications of Oxidized Nanocarbons: from Catalysis to Nanocomposites

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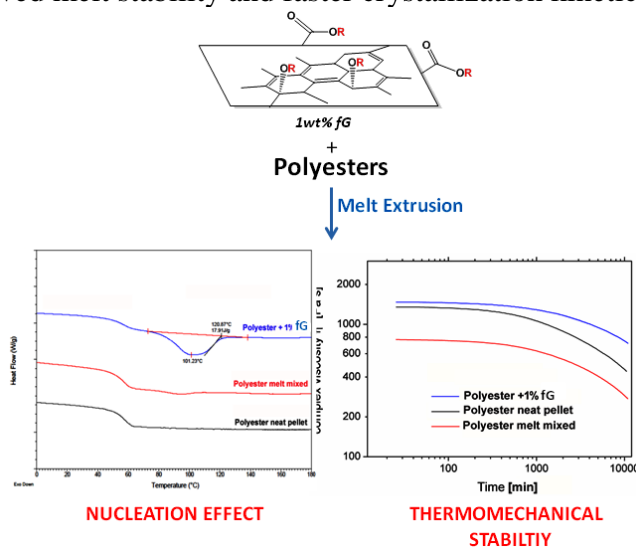
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Oxidized Nanocarbons, mainly regarding Graphite Oxide (GO) and Oxidized Carbon Black (oCB) are 2D carbon nanostructures containing many hydrophilic groups, making them promising in many potential applications. In particular, GO and oCB has recently been used both as catalyst for important organic reactions (1-4) and as filler of polymers (5-7).

The first part of the contribution will describe preparation and use of oxidized nanocarbons, their ability to catalyze some important reactions and how this catalytic activity can be technologically relevant for polymeric matrices, mainly regarding epoxide and phenolic resins.

The second part of the contribution will be devoted to the incorporation of carbon nanofillers in several commercial biodegradable polyesters. In particular in this study we will show that the incorporation of oxidized nanocarbons induce polymer degradation during melt processing. On the contrary, their covalent functionalization minimizes polymer degradation in melt processing, thus allowing the production of polyesters/graphite-based nanocomposites. Furthermore, a nucleation effect was observed able to increase the crystallization kinetic ten times more than the usual filler. We carried out functionalization of GO (fG) and oCB (fG) by introduction of alkyl groups by a well-known methodology (8) and acetyl groups by a new green procedure (9). With both functionalizations, improved melt stability and faster crystallization kinetic were achieved.



Nucleation effect and thermomechanical stability in biodegradable polyester/fG nanocomposites

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Vibrational spectroscopy investigations on graphene/Poly (lactic acid) composites

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Poly (lactic acid) (PLA), a biodegradable and biocompatible polymer, is suitable for food packaging, medical applications and implant devices. However, its applications are limited by intrinsic drawbacks including slow crystallization rate, low thermal stability, relatively poor mechanical and barrier properties. Adding nano-sized fillers provides a way to improve the performances of PLA and to expand the its applications. (1) To this aim, PLA based films containing low amounts (up to 0.75 wt %) of graphene nanoplatelets (GnPs) were prepared by a solvent casting procedure and characterized by vibrational spectroscopy. (2) Confocal Raman Imaging provided information on the distribution of GnPs taking advantage of the high spectroscopic contrast, the appropriate space resolution and sensitivity. In fact, the experiments carried out by this technique highlighted the presence of well-defined domains ($\approx 15 \mu\text{m}$) for PLA loaded at 0.25% wt (figure 1); while, at higher GnPs content (0.75 % wt) a co-continuous phase is distinguishable in the whole sample.

In-situ FTIR spectroscopy was used to study the diffusion of water vapor in pristine and in GnP modified films. It was demonstrated that the solubility and the diffusivity of H₂O vapor decrease appreciably by increasing the GnP content in the composite. The *time-resolved* spectra, analyzed by different techniques (difference spectroscopy, DS, least-squared curve fitting, LSCF and 2D correlation spectroscopy, 2D-COS) provided relevant and complementary information on the diffusion mechanism and the molecular interactions occurring between the penetrant and the polymeric host.

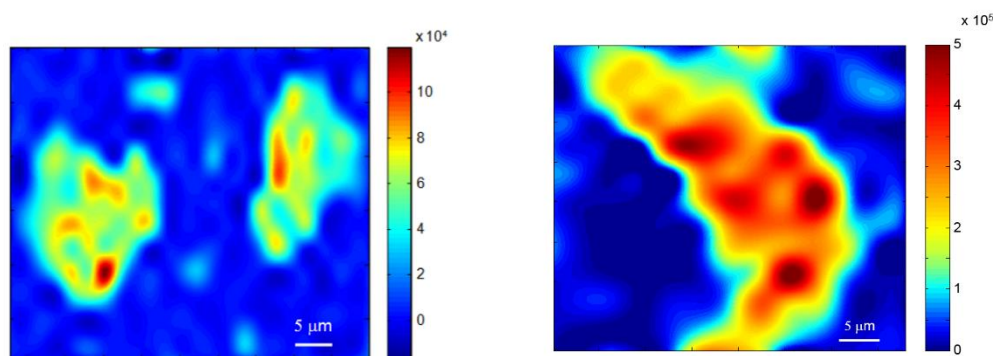


Figure 1. Confocal Raman Imaging of PLA/GnPs 0.25 wt % (left) and PLA/GnPs 0.75 wt % (right)

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Porous graphene-based polyurethane foams-aerogel composites prepared via unidirectional freeze-drying process

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Carbon based aerogels exhibit excellent properties, such as low density, high conductivity, outstanding adsorptive property. However, in most cases carbon aerogels are mechanically fragile and show poor resilience, which limit their applications. In this work, a novel complex structure with high electrical conductivity was designed based on open cell polyurethane foams (PUF) and reduced graphene oxide (rGO)/chitosan (CS) aerogel. The lightweight, highly porous, electrically conductive rGO/CS aerogel was formed in-situ within the PUF porous structure via unidirectional freeze-drying technique. The resulting structure is illustrated in Figure 1. As an integrated structure the aerogel was mechanically supported by the elastic PUF scaffold. However the conductive 3D network constructed by aerogel offered a robust conductive network throughout the whole material. Therefore this structure possess many unique features, such as good mechanical properties, excellent electrical conductivity and outstanding piezoresistive properties. To enhance the interface bonding, the PUF surface was coated by an rGO coating layer through liquid phase deposition process. The influence of rGO coating layer on the mechanical and electrical properties was investigated. The electrical properties in the parallel and transverse directions of aerogel growth are reported. This study provides a novel alternative approach to preparing high performance polymer nanocomposites with potential application prospects in many fields, including wearable sensors, catalyst carriers and adsorbent materials.

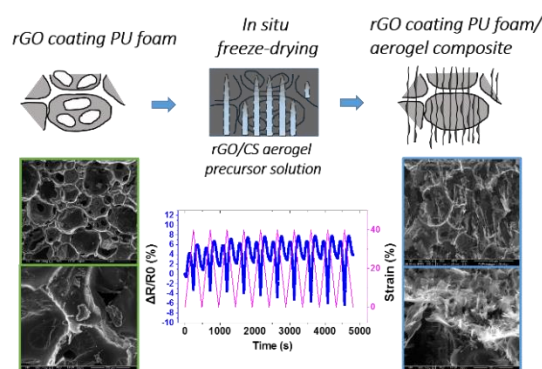


Figure 1: SEM images and stable piezoresistive property of the novel structure resulting from the *in-situ* formation of reduced graphene oxide/chitosan aerogel in the open cell polyurethane foam.

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Multifunctional properties of Graphene Nanoplatelets based nanolaminates

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Among the different composite architectures, nanolaminates are emerging as interesting materials for structural and functional applications. Nanolaminates is a biomimetic architecture copying the structure of nacre consisting of the assemblies of well-oriented nanolaminae held together by an extremely low content of matrix. Nanolaminates consists of a stiff constituent phases bonded together by the soft constituent phases resulting in the so-called ‘brick-and- mortar’ (‘B-and- M’) structure. The combination of a small fraction of polymeric phase along with the nanolaminate three-dimensional architecture leads to exceptional mechanical properties, including high toughness, high strength and high stiffness. (1, 2, 3, 4)

We have developed nanolaminates containing very high content (>80% w/w) of graphene nanoplatelets, GNP, within an uncured epoxy matrix (prepregs) that are suitable for the conventional prepregs manufacturing technologies: film stacking and consolidation under temperature under pressure. Such kind of materials shows exceptionally rich multifunctional properties. See Table 1. Such as high and anisotropic thermal and electrical conductivities, low density, high Young modulus and damping capacity, very low Water Vapor Transmission Rate, fire resistance (in terms of flame retardation and reduction of the peak emission), high electromagnetic shielding and IR mirroring. In addition, the flexible manufacturing route enables an easy interchange of the polymeric matrix: GNP nanolaminated sheets (A3 dimensions) have been manufactured with both thermoset and thermoplastic polymer matrices.

Several industrial applications are in the development stage that take advantages from the multi functionality of the GNP nanolaminates, among the others: flexible batteries, fire protection systems and bulk graphite substitution in high temperature ovens.

Work is in progress to further dope the nanolaminate composition to access new functional properties, for example the addition of metallic nanoparticles to increase the peak electrical current before material break down.

Thickness (µm)	50	
Max. Sheet size (mm)	400x400	
Density (g/cm ³)	1,2 – 1,8	
Thermal conductivity (W/mK)	X, Y direction	> 1600
	Z direction	50
Specific Heat @ 25°C (J/g°K)	0,8	
Thermal diffusivity (cm ² /s)	14 - 16	
Sheet Resistance (Ohm/sq.)	0,2	
Electrical conductivity (S/m)	10 ⁵	
Bending (Cycles)	> 10000	
Storage Modulus (GPa)	26	
Loss Factor	0,03	
Fracture Toughness (MPa)	37	
WVTR (HR 50%) (g/(m ² -day)	1,2	
WVTR (HR 75%) (g/(m ² -day)	1,6	
EMI Shielding (dB)	70	
Heat Resistance (°C)	200 - 500	
Fire Resistance	pHRR (KW/m ²)	-39%*
	THR (MJ/m ²)	-31%*
	TTI (sec)	+180%*
	TSP (m ²)	-58%*
	TSR (m ² /m ²)	-58%*
RoHS compliant	√	

*Percentage improvement respect to CFRP

Table 1
Properties of GNP nanolaminates

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Formulazioni nell'Industria Chimica e Farmaceutica

Formulations in the Chemical and Pharmaceutical Industry

Formulation and Specialty Chemistry: the needs of Chemical Industries

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In the Specialty Chemistry, Italian industry has developed a true specialization that deriving from the characteristics of the companies, the interaction with the users of the Made in Italy and industrial districts.

The results of this specialization are evident in foreign trade data showing a growing active balance that has now exceeded € 3 billion.

Key success factors were: flexibility, creativity and innovation ready to offer quality solutions to the user.

Nowadays, the challenges of the global market lead the industry (not just the large companies) to an increase in terms of quality towards more and more structured research. To be able to contribute significantly to the competitiveness of downstream productions, the Specialty Chemistry has to offer not only fast responses but also anticipate needs with a design that must also produce patents.

The strong links between chemical industry and chemical science find in this context the need for chemistry of formulas to have a growing role in the university programs, in the forms that Universities can identify according to their characteristics and needs of the territory.

The drive towards research involves the need for well-prepared chemists in the areas of industrial specialization, bearing in mind that the size of the companies does not always allow the company to act in a proactive way. This action should be done by universities also by promoting Thesis of industrial interest.

Formulation challenges and emerging technologies in the pharmaceutical industry: an overview

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Quality and innovation are two of the pharmaceutical industry's most defining characteristics. They are the driver for profitable revenue growth and long-term sustainability. Now more than ever, partnership and collaboration are essential to advance drug delivery innovation. This is due to several factors:

- Increasing complexity of both small- and large-molecule drugs;
- Increasing consumption of medicines in both emerging and mature markets;
- Growing number of biologic drugs in development;
- Entrance of several small startups into the market;
- Increasing generic competition.

As the pharmaceutical industry continues to move towards a quality-by-design (QbD) paradigm, the design and control of the Active Pharmaceutical Ingredients physico-chemical properties as well as the demonstration of greater understanding of the development of the Drug Product and its manufacturing process become an area of increasing interest.

Some of the key formulation challenges and emerging technologies in the pharmaceutical industry include:

- Delivery/oral delivery of biologics;
- Poor solubility;
- Patient-friendly drug delivery and packaging systems;
- Personalized medicines;
- Pediatric formulations;
- 3D printing;
- Nanotechnology;
- Drug discovery by design;
- Gene delivery;
- Advanced Therapy Medicinal Products (ATMP);
- Antibody-Drug Conjugates (ADC);
- QbD, Process Analytical Technology (PAT) and Manufacturing Excellence;
- Continuous Manufacturing (CM);
- Manufacturing Classification System (MCS) for oral dosage forms;
- Classification of Direct Compression (DC) excipients;
- Biopharmaceutics Classification System (BCS), Developability Classification System (DCS), Biopharmaceutics Drug Disposition Classification System (BDDCS), Extended Clearance Concept Classification System (ECCCS) in drug discovery and development settings.

This list (which is far from being exhaustive) groups both quality- and technology-related aspects. The former are indicating a trend towards the categorization of the formulation activities and manufacturing processes, possibly reflecting the high growth rates for contract manufacturing. The latter represent either emerging or relatively consolidated tools intended to provide solutions to ensure high bioavailability, efficacy and safety of today more complex candidate drugs.

A few selected examples of either group will be given in this presentation.

Formulation Chemistry: a new frontier of the Chemistry in Italy

Sesto Viticoli^a

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Chemistry has been largely identified over the years just with chemical products as individual chemical species characterized by their production processes and their use for specific chemical and physical properties. The ability to use individual chemicals can be significantly expanded and improved if they are physically combined to achieve otherwise unattainable properties or to achieve a desirable cost advantage. In this respect, Formulation Chemistry play an important role for several areas of particular interest National Companies such as, for example, Health, Agri-Food, Construction, and Industry's heterogeneous and photo-sensitive systems.

By way of example (1) we can cite, for heterogeneous systems, the case of tires where, by introducing polar functional groups on polymer chains into silica-containing compounds, an improved effect on the dissipative properties of the material, resistance to tire rolling and therefore fuel consumption of the vehicle. The same statement applies to Construction, where new Formulations are designed to follow and possibly anticipate the evolutionary trend of new market needs, such as new functionality and multifunctionality of materials, durability and sustainability, to control the structure of matter at nanometric scale and identify the material degradation mechanisms, to develop the market for new nano-structured products, eg. in the field of prefabricated elements.

Formulations play a central role also in modern Agriculture, especially in terms of modulating the release of active ingredients in a controlled way over time; reducing the level of assets in the environment, also controlling degradation; eliminating the exposure to toxic substances by operators; increasing the photostability of the active substances, thus reducing the amount of pesticides placed into the environment.

In the field of the drug, the Formulations strongly affect three parameters such as speed, time and place, which are essential to control and modify the drug release mechanisms. The Wellness can become a very promising area in relation to the new needs of consumers, industrial needs, the advancement of scientific knowledge and the development of new analytical techniques, the evolving international standards increasingly vigilant Public health and consumer protection. These development parameters must be added to the extreme dynamism of a sector that has a very high turn-over in products, both in terms of new proposals and the average life expectancy of traditional products. Cosmetic ingredients also have a high index of innovation, with the annual input of over 300 new raw materials (mostly blends), both synthesis and extraction or natural derivation, to increase their nutraceutical properties and give rise to a nouca Area defined as Cosmeceutica (Cosmetics + Nutraceuticals).

Trimbow[®] a new extrafine triple combination in a single inhaler for COPD treatment

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After 60 years from the first commercialization of a pressurized metered dose inhaler (pMDI) by Riker Laboratories in 1956 (later acquired by 3M Pharmaceuticals) this pharmaceutical form remains a common and extensively used method to treat lung diseases such as asthma and Chronic Obstructive Pulmonary Disease (COPD). Medical treatment of lung disease has changed significantly over time pushing the drug maker to develop new treatments, which can better address the patient needs. In this scenario many patients with COPD are recommended to use combination therapy composed of bronchodilators such as β_2 agonists and long acting muscarinic antagonists (M_3 antagonist), and anti-inflammatory agents like inhaled corticosteroids (ICS).⁽¹⁾ Patients with COPD receiving such triple therapy currently use at least two inhalers, typically an ICS plus a long-acting β_2 -agonist combination in one inhaler and a long-acting muscarinic antagonist in a second, and often these inhalers are of different types and designs which may affect patient compliance⁽²⁾. The therapeutic gap has been recently filled by Chiesi Farmaceutici which has developed a novel triple fixed dose combination (Trimbow[®]) in a single inhaler (pMDI) containing formoterol fumarate (B_2 agonist), glycopyrronium bromide (M_3 antagonist) and beclometasone dipropionate (ICS), which has recently been approved in Europe.

The development of multi-drug containing products is very challenging and involves a very high level of technical, clinical and regulatory requirements, which discourage the development of such pharmaceutical forms. The safety and efficacy of the fixed dose combination should be demonstrated against its single and double combination components, whilst technically the combination of the three active ingredients involves a significant effort in the design and formulation development in order to assure the quality of the final product in terms of delivery performance and chemical-physical stability. The Trimbow[®] development approach addressed all the hurdles by means of an extensive technical, pre-clinical and clinical program to assess the safety and efficacy by means of 12 different clinical studies involving more than 7000 patients. Trimbow[®] formulation was developed under the Chiesi Modulite[®] technology platform as a pMDI solution with the goal of having an extrafine product (i.e., mean mass aerodynamic diameter (MMAD) $<2.0 \mu\text{m}$)⁽³⁾. The extrafine formulation enables efficient lung deposition allowing an optimal distribution of the active ingredients both in the central and peripheral lung⁽³⁾. Despite achieving the typical dose reproducibility and the optimal low particle size of the emitted dose from a pMDI solution, it is known that the chemical stability of the active ingredients could be critical especially when more than one active ingredient is combined in the same inhaler. The concept of combining different bronchodilators with an ICS in a single inhaler is therefore an attractive opportunity to minimize the number of medications that the patient should take on a daily basis and thus may enhance patient compliance. Thus, few Triple fixed combination therapies are currently in late stage development/available in the world⁽⁴⁾ and none of the them are pMDI solutions or can claim to be extrafine products. Despite of the technical challenges, Chiesi was able to develop a formulation capable of assuring the chemical stability of the three active ingredients with the desired product performance becoming the first company to gain approval for a Triple fixed combination therapy in Europe.

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Study of the nanostructure of innovative formulations for cement mixtures

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Water is the main source of the premature deterioration of concrete structures, by carrying dissolved aggressive chemicals such as chloride and sulfate ions into the concrete structure, which can cause the corrosion of steel rebars and the expansion of concrete paste due to delayed ettringite formation. The critical factors that contribute to the durability of concrete are a dense microstructure, a fine pore structure and low capillary porosity (1). The addition of supplementary cementing materials (SCMs) into concrete mixtures has been gaining acceptance with respect to improving durability and reducing permeability (2). In addition, a class of materials referred to as permeability-reducing admixtures (PRAs) have been developed to improve concrete durability by reducing the permeability of cement paste of concrete (3).

This paper describes a new concrete permeability reducing admixture capable to effectively reduce the movement of water under hydrostatic head pressure (PRAH). The new admixture is an aqueous suspension of nano-sized metal transition polymeric silicate hydrate that catalyzes the nucleation of CSH in the capillary pores of hydrating cement paste. The crystallization of CSH in the capillary pores refines the capillary porosity of cement paste and significantly increases the resistance to water penetration under pressure. The mechanism of homogeneous crystallization of CSH was demonstrated by Synchrotron XRD micro-Tomography (XRD- μ T) and by Scanning Electron Microscope (SEM) investigations. The effectiveness of the new admixture was tested on concrete specimens by measuring the water permeability according to European Standard EN 12390-8. The results indicated that the new admixture is highly effective in reducing the penetration of water, compared to a reference concrete with the same W/C and to other PRAH admixtures, working with different mechanisms. The new admixture also increases the early strength development of concrete and can be used in conjunction with WR and HRWR to produce concrete with outstanding mechanical performances and durability.

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Innovative approaches to tailor a particle size distribution

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In the pharmaceutical industry, size reduction techniques are used to improve powder processing and to increase, when solubility is the limiting step, the bioavailability of an active pharmaceutical ingredient (API) to obtain the desired therapeutic effect or to aid in drug product formulation.

One common size reduction technique used by the pharmaceutical industry is jet milling. With this technique, comminution is based on a particle-to-particle collisions mechanism that avoids the use of moving parts and the consequent risk of foreign particles contamination.

Grinding nozzles allow the grinding gas to enter at supersonic speed into the grinding chamber creating a vortex of gas that accelerates the powder particles within a spiral flow path inside the grinding chamber.

Centrifugal force directs particles to the outside of the chamber, while an opposite drag force is created by the gas exiting the milling chamber and forces the particle through a central exit.

As centrifugal force is proportional to the particle diameter cubed and drag force is proportional to the particle diameter squared, as particles break into smaller fragments the centrifugal force decreases faster than the drag force. Once the drag force on the particle exceeds the centrifugal force, the particle is brought out of the milling chamber.

To influence the resulting particle size created during the process, the typical operating variables are: grinding pressure, feeding pressure, and feed rate.

When the modifications of the previously mentioned variables do not lead to the desired PSD it is possible to act on the geometrical parameters of the jet-mill as: grinding chamber dimensions and shape, nozzles diameter and angle, static classification system diameter and length etc...

Unfortunately, also applying all the possible geometrical variations, it is impossible to precisely control the amount of fine fraction leaving the milling chamber. This means that over a certain value, there will be a limited control of the PSD dispersion.

In this case, one of the available option is to couple the jet-mill with a dynamic classification system to separate the unwanted fraction from the PSD.

With this solution, the product exiting from the jet-mill is fed into a classification chamber where the powder is accelerated against a classifier wheel. At this stage, fines are separated from oversize and subsequently routed for collection. Feed rate, air flow and rotor speed can be adjusted to vary the “cut size” of the fractions that will be collected before and after the dynamic classifier.

I cosmetici per pelli sensibili: strategie formulative per la modulazione dell'attività lenitiva ed anti-infiammatoria

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La sensibilità cutanea e le manifestazioni infiammatorie sono problematiche con una incidenza epidemiologica molto elevata ed in progressivo aumento. I soggetti con pelle sensibile rappresentano in Europa e negli USA circa il 60% del mondo femminile ed il 40% del mondo maschile. Il claim “sensitive skin” coinvolge il 25% dei prodotti cosmetici sul mercato (Mintel's Global New Products Database 2017). In campo dermatologico i fenomeni infiammatori accompagnano le dermatiti (allergiche, irritative, atopiche, seborroiche, foto-indotte) e gli eczemi cutanei. La cute, infatti, è l'organo umano più esteso, in perenne contatto con l'ambiente esterno e svolge un ruolo primario nella difesa immunitaria dell'organismo. Le citochine dell'epidermide possono avere un ruolo importante nel mediare il processo infiammatorio e la risposta immunitaria della cute. Negli ultimi anni molti cosmetici specifici per le pelli sensibili e reattive sono stati sviluppati ed immessi sul mercato, privilegiando principi funzionali di origine naturale. Gli estratti dalle radici della *Glycyrrhiza glabra* contengono composti storicamente utilizzati per le proprietà di modulazione dei fenomeni infiammatori cutanei (1). Le proprietà biologiche di questa pianta sono associate alla presenza della glicirrizina e del suo aglicone l'acido glicirretico. Alcuni derivati come il dipotassio glicirrizinato (DG) e lo stearil diglicirrizinato (SG) sono utilizzati in preparati per uso esterno: in preparati cosmetici per le proprietà lenitive anti-rossore (2) ed in preparati ad uso dermatologico per migliorare la sintomatologia delle dermatiti sia acute che croniche. DG e SG hanno una elevata stabilità chimica ma differenti proprietà chimico-fisiche e solubilità. Infatti mentre DG ha una buona solubilità in acqua, SG ha un pronunciato carattere lipofilo. Queste caratteristiche sembrerebbero rendere tali sostanze non facilmente biodisponibili in quanto le sostanze molto idrofile o lipofile sono normalmente non ben assorbite per via transcutanea (3). Lo scopo dello studio condotto è stato quello di valutare la capacità di veicoli differenti (emulsioni O/W e gel) e di penetration enhancers nel modulare l'assorbimento percutaneo di DG ed SG. Inoltre si è valutata in parallelo la capacità veicolante di sistemi micro-particellari (4) quali Solid Lipid Nanoparticles (SLN). L'assorbimento percutaneo è stato studiato in vitro (5) utilizzando membrane strato corneo-epidermide (SCE) in celle di Franz. In vivo è stata poi determinata la proprietà anti-infiammatoria (6). Dai risultati ottenuti si evidenzia, per quanto riguarda la forma tecnica del veicolo, come il gel promuova meglio l'assorbimento di DG e l'emulsione O/W l'assorbimento di SG. Dai risultati ottenuti, inoltre si evidenzia, come l'utilizzo di penetration enhancers o di SLN, rappresenti una tecnologia valida per l'ottimizzazione del rilascio topico di DG ed SG. In particolare, l'uso di lecitina di soia idrogenata consente un aumento dell'assorbimento percutaneo dei due attivi ed un effetto antiinfiammatorio che si esplica a tempi brevi post applicazione nei test in vivo. Le SLN cariche di SG hanno invece evidenziato una “sustained and delayed” attività infiammatoria.

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Challenges in formulating Ace Bleach products

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Fater Research and Development department proudly defines its mission as “the magic behind the promise of our brands”. This magic consists in three activities that constitute the essence of R&D:

- “Translate” the Promise turning consumer needs and brand benefits into product/package measurable attributes
- Make the Promise “real” identifying enabling technologies, and designing products and packages which delight consumers at affordable costs
- Keep the Promise by designing and scaling up manufacturing process which can deliver quality products & packs, day in day out

With focus on formulation challenges and approaches to problem solving, the presentation will provide specific examples of:

- How Fater R&D designs a cleaning product based on consumer needs
- Approaches to formula design to maximize performance
- Formula stability studies for intrinsically unstable bleach-based products

Founded in 1958, since 1992 Fater is an equal share joint venture between the Angelini Group and Procter&Gamble.

For more than 50 years Fater has presence in Italian homes through its products: Pampers, LINES, TAMPAX, LINIDOR and DIGNITY. Since 2013, Fater acquired the ACE brand, expanding its line of brands.

A rare example of successful joint venture over a long period of time, Fater bases its growth on its in-depth knowledge of consumers and markets, combined with the application of multinational work methods.

Fater is a dynamic company that believes in continuous innovation and it invests 4% of its turnover in Research&Development.

Fater Headquarter is located in Pescara, we have several affiliates in Moscow, Bucharest, Istanbul and Mohammedia and manufacturing plants in Italy (Pescara and Campochiaro), in Portugal (Porto), in Turkey (Gebze) and Morocco (Mohammedia).

Fater counts globally 1,400 employees and 915 million Euros of turnover (ref. 2013/2014 financial statements).

Formulazioni nel settore della nutraceutica: stato dell'arte e prospettive future

Antonino Bagnulo

Shedir Pharma

Colloids and Nanosciences: Formulations and New Challenges

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Colloidal systems are crucial to many materials broadly used in everyday life (such as plastics, pharmaceuticals, cosmetics, agrochemicals, paper, food, inks, paints, detergents, cements, and many others). The number and variety of potential applications clearly highlight the importance of colloids in the field of formulations, but also denotes its multidisciplinary nature, requiring the combination of multiple skills and the knowledge of chemistry, physics, biology, engineering and medicine. Furthermore, over the last couple of decades, the advances in the field of nanosciences have made available to both academic and industrial researchers a plethora of nanostructured materials and innovative technologies that could be integrated within commercial products to improve their quality and to optimize their production costs, as well as to design completely new products.

In such a crowded and challenging scenario, it is now obvious that the cooperative connection between academia and industry is a pre-requisite for excellence in the field of formulations. In this contribution, we will report on examples where the scientific collaboration between industrial partners and the CSGI consortium has taken to the formulation of commercially relevant materials based on colloids and nanostructured materials.

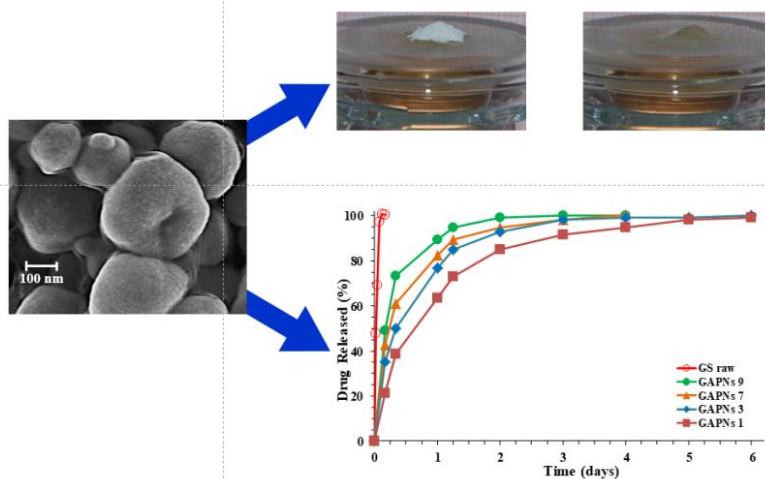
Polysaccharides based in situ gelling powders as promising wound healing medical devices

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Injury to the skin provides a unique challenge, as wound healing is a complex, sequential and intricate process. Acute wounds have the potential to move to chronic wounds, which are arrested in a specific phase of wound healing and unable to progress. There is tremendous pressure on the medical system to develop new and cost-effective therapies due to high cost of the treatments as well as associated health care system and social costs. Wound care as well as wound management products are essentially aimed at ensuring wound healing and infection control. Their effectiveness is can be measured by incidence of complete closure and quality of healing, by prevention or treatment of infection, reduced pain and reduced blood loss during debridement. A number of wound care products are available on the market and approved as over-the-counter (OTC), prescription topical products and medical devices. Still there is no device that can be configured as an optimal product due to the many technical challenges associated to the development of the ideal device. In fact, an ideal device should avoid local irritation and contact sensitization as well as immune reactions, dehydration of the wound site and removal trauma. Moreover, it should be cheap in order to reduce treatment costs. Therefore, the need of innovative products is very high, owing the unsatisfying clinical outcomes and low effectiveness of many conventional products.

In order to overcome such problems an innovative product consisting of polysaccharides blend submicrometric powder, able to form in situ a soft gel dressing when in contact with exudates, have been designed in our lab. Alginate, pectin and chitosan with specific molecular weight and moieties have been used as excipients to prepare the powder that have been used as carrier for different active ingredients (i.e. antibiotics, NSAIDs, and peptides). Nanospray drying technique has been chosen as encapsulation technology to produce the drug loaded powder due to the possibility to run the atomization process at low temperature (50-60 °C) and high processes yield (> 85%). Submicrometric particles show narrow size distribution, spherical morphology, smooth surface and good flowability. The proper polysaccharide blend used to make the particles is able to move the powder from solid to gel state very quickly (5-15 min) when in contact with wound fluids, producing a gel barrier able to fill completely the wound cavity. Moreover, the polysaccharide blend gel has demonstrated high fluid uptake ability (between 10 and 15-fold its dry weight) resulting in high exudate absorbance from wound bed and proper adhesiveness to the wound due to the formation of highly entangled gel texture during the submicrometric particles swelling. The entanglement of the *in situ* formed gel is also able to control the release of the loaded drug prolonging its release (between 1 – 12 days) depending on drug/polymer blend ratio and physico-chemical properties of the loaded active ingredient.



Industrial Formulation: a new curriculum in Industrial Chemistry Master's degree

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The Department of Chemical Sciences of University of Naples Federico II has made a careful analysis of the evolution of the Italian chemical industry, to improve and increase the attractiveness of the Master's Degree in Industrial Chemistry.

Particularly interesting were data reported in the Report of the Italian Association for Industrial Research (AIRI) on Priority Technologies of Industry (1). In the chapter dedicated to the chemical industry, it is emphasized that that formulation technologies involve about 70% of Italian chemical and pharmaceutical industry, and as a consequence there are a strong need for research and training in the formulation sector.

It is clear from the above that activating a curriculum devoted to the formulation would surely find a strong interest in Italian industrial sector. However, to have a high quality training, it is necessary to have the skills.

An analysis was then carried out to evaluate the activities that the Department of Chemical Sciences has done over the past 10 years, identifying activities related to the formulation sector. The analysis showed that an intense activity has been done in the field of formulation and in many cases these activity has been done in collaboration with Industry.

A new curriculum has been designed by activating 4 courses devoted to the formulation science and technology for a total of 24 CFU. Then, the formation of the students will be deepened during the thesis (38 CFU) that will be dedicated to the formulation sector.

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