Società Chimica Italiana
Divisione di Chimica
Industriale

ATTI DEL CONGRESSO

XXII CONGRESSO NAZIONALE DELLA DIVISIONE DI CHIMICA INDUSTRIALE

7-8 NOVEMBRE 2022 | CATANIA

a cura del Comitato Organizzatore

PREFAZIONE

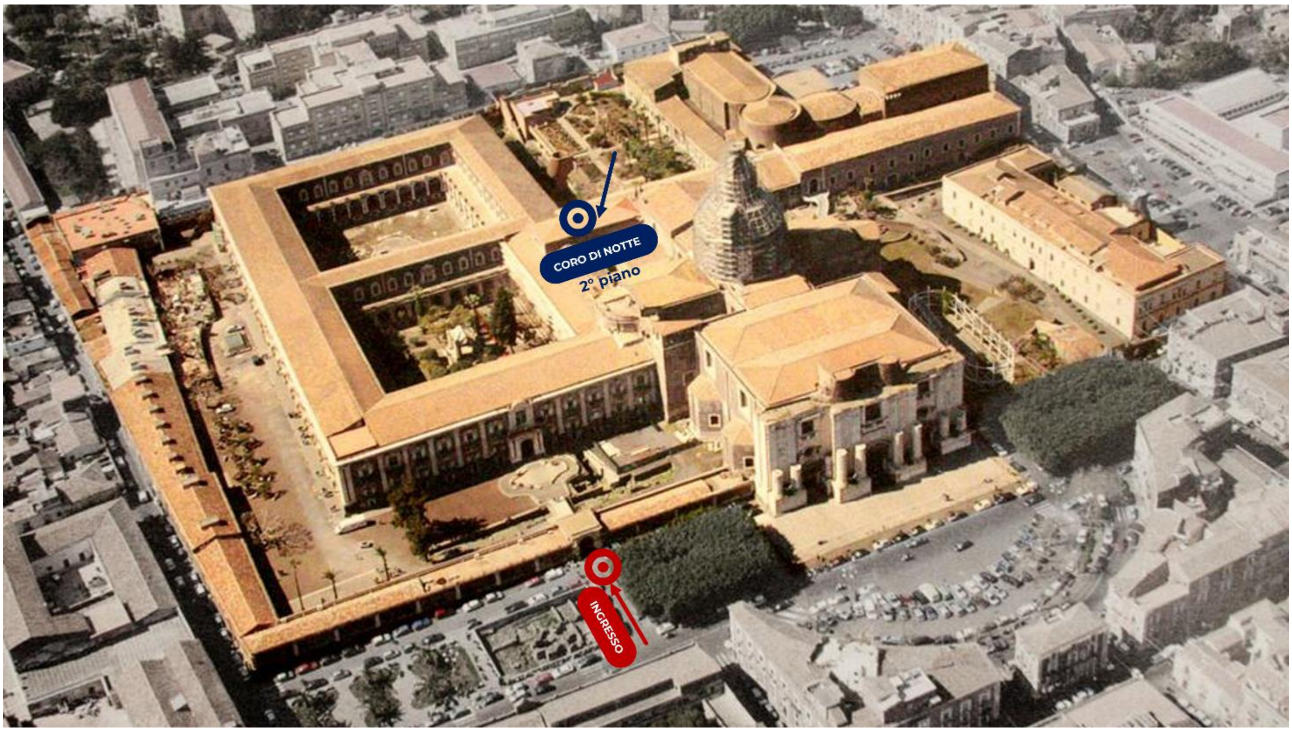
Il XXII Congresso Nazionale della Divisione di Chimica Industriale della Società Chimica Italiana si svolgerà a Catania nel Monastero dei Benedettini nei giorni 7 e 8 novembre 2022.

Le tematiche scientifiche oggetto del Congresso riguardano tutti i temi cardine della Chimica Industriale (sviluppo di prodotti chimici, materiali, polimeri e processi catalitici) e le relative applicazioni, con particolare attenzione agli aspetti della sostenibilità e dell'economia circolare.

Come da tradizione, il congresso vuole essere un momento di incontro tra il mondo dell'accademia e quello dell'industria, dove si possano confrontare domanda e offerta di innovazione nei settori strategici della Chimica Industriale.

SEDE DEL CONGRESSO

Il Congresso avrà luogo nel Monastero dei Benedettini, sito in Piazza Dante 32, oggi una delle sedi dell'Università degli Studi di Catania. I lavori Congressuali si svolgeranno nell'Aula "Coro di Notte", sita al secondo piano, al centro del vecchio complesso monastico (vedi mappa). Il Monastero è uno dei plessi monastici più grandi d'Europa, un luogo unico che racconta le vicende umane e storiche della città dell'Etna dall'antichità fino ai giorni nostri.



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PROGRAMMA SCIENTIFICO

Lunedì 7 novembre 2022

08:30 Registrazione

Apertura lavori - Saluti e ringraziamenti
Mario Marchionna, Presidente Comitato Scientifico
Siglinda Perathoner, Presidente Comitato Organizzatore
Salvatore Scirè, Comitato Organizzatore Locale

Sessione Premi e Medaglie
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Gabriele Galletti – Università di Bologna
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Luca Mastroianni – Università degli Studi di Napoli Federico II
P18: *Oxidation of Alcohols Promoted by Gold in a Microreactor: Kinetic and Modeling Study*

10:00–10:30 **Medaglia Chiusoli**
Matteo Maestri – Politecnico di Milano
Unraveling the nature and the identity of the active site in heterogeneous catalysis by a structure-dependent multi-scale and multi-technique approach

10:30–11:00 **Medaglia Giacomo Levi**
Alessandro Trovarelli – Università di Udine
Amod Sagar – Treibacher Industrie AG
Development of Novel Materials for Exhaust Gas Catalysis

11:00–11:10 **Premio Miglior Tesi di Dottorato 2022**
Angelo Nicosia – Università di Catania
Polymer-based Graphene Oxide Derivatives as tunable multipurpose platforms

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Chair **Martino Di Serio**

11:40–13:30 **Approcci Industriali**
Sessione Scientifica I
O1: **Giorgio Ferrari** – Mapei S.p.A.
Low Carbon Concrete Admixtures – LCCAs

O2: **Daniele Martella** – Istituto Nazionale di Ricerca Metrologica
Photoresponsive polymers for smart adhesives and surfaces

O3: **Andrea Pucci** – Università di Pisa
Luminescent Solar Concentrators with Outstanding Optical Properties: Cell-Casting and Scaling-Up

O4: **Ilenia Rossetti** – Università degli Studi di Milano
Conceptual design of a process for the use of liquid ammonia as hydrogen vector

O5: **Massimo Innocenti** – Università di Firenze
New industrial processes with low environmental impact in the energy and electrodeposition sectors

O6: **Arian Grainca** – Università degli Studi Milano
Hazard and operability (HAZOP) application in a Fischer-Tropsch laboratory scale

O7: **Luca Rosi** – Università di Firenze
Microwave pyrolysis of waste plastics
An overview of the activities at the University of Florence

O8: **Michele Casiello** – Università degli Studi di Bari
Clays as catalysts in biodiesel production from waste lipids

13:30–14:30 Light Lunch

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Flexible platforms for functional additives in industrial applications

Chair **Michela Signoretto**

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Photocatalytic and photoelectrocatalytic H_2 *prduction by furfuryl alcohol reforming*

O10: **Stefano Andrea Balsamo** – Università di Catania
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Development of perovskite-based materials for the photo-catalytic valorization of CO_2

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Innovative floating photocatalysts for wastewater remediation: a fascinating world merging environmental protection and circular economy

O15: **Luca Spitaleri** – Università di Catania
ZnO@Au Core-Shell Nanoparticles as Efficient Photocatalysts for Photocatalytic Oxidation of VOCs in Air Purification

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Chair **Daniele Caretti**

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O17: **Alice Capitti** – Università di Firenze
Biopolymers from biomass valorization towards new functional materials

O18: **Sandro Dattilo** – CNR-IPCB SS Catania
Cryogels platform for the removal of emerging pollutants

O19: **Simone Galliano** – Università degli Studi di Torino
Improved sustainability of thermosetting polyurethanes with Design of Experiment

O20: **Massimo Bernardini** – Università degli Studi di Genova
Influence of the addition of plastic waste residues in coal blends for coke production

O21: **Lidia Mezzina** – Università di Catania
Photosensitized Thermoplastic Nano-Photocatalyst for Potential Applications in Extraterrestrial Facilities

O22: **Matteo Gastaldi** – Politecnico di Torino
3D printed light-activated polymer

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Chair **Stefania Albonetti**

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O24: **Francesco Taddeo** – Università di Napoli Federico II
Kinetics of Levulinic acid esterification with ethanol: from batch to continuous operation

O25: **Francesco Prandi** – Università di Bologna
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O26: **Maela Manzoli** – Università degli Studi di Torino
Microwave-assisted reductive amination of aldehydes and ketones over Rh-based heterogeneous catalysts

O27: **Stefano Scurti** – Università di Bologna
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O28: **Michele Emanuele Fortunato** – Università di Napoli Federico II
Synthesis of methyl-levulinate catalyzed by an ion-exchange resin: a kinetic investigation

O29: **Ludovica Di Lorenzo** – Università degli Studi di Torino
Acrylic pressure-sensitive adhesives A "green" chemistry route

O30: **Elena Spennati** – Università degli Studi di Genova
Co-based catalysts for CO_2 hydrogenation: methanation vs. reverse water gas shift activity

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Chair **Anna Maria Raspolli Galletti**

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O31: **Marcello Pagliero** – Università degli Studi di Genova
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O32: **Federica De Luca** – Università degli Studi di Messina
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O33: **Ilaria Rizzardi** – Università degli Studi di Genova
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O34: **Camilla Parmeggiani** – Università di Firenze
Smart materials based on liquid crystals for tissue engineering

O35: **Tiziana Avola** – Università degli Studi di Milano
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O36: **Alessandro Di Michele** – Università degli Studi di Perugia
Sonochemical synthesis of iron based nano-hydrotalcites promoted with Cu and K as catalysts for Fischer-Tropsch synthesis in biomass to liquid process

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PARTECIPANTI

Salvatore Abate
Stefania Albonetti
Claudio Ampelli
Claudia Antonetti
Sara Aquilia
Maria Teresa Armeli
Tiziana Avola
Stefano Andrea Balsamo
Marianna Bellardita
Edmondo Maria Benetti
Massimo Bernardini
Monica Bertoldo
Martina Buccioli
Marta Calà Pizzapilo
Alice Cappitti
Daniele Caretti
Michele Casiello
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Gabriele Galletti
Simone Galliano
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Riccardo Gallorini
Gabriella Garbarino
Matteo Gastaldi
Davide Gazzi
Elena Ghedini
Arian Grainca
Gaetano Iaquaniello
Massimo Innocenti
Eleonora La Greca
Domenico Licursi
Leonarda Francesca Liotta
Simone Livolsi
Francesca Lorandi
Matteo Maestri
Eleonora Manarin
Maela Manzoli
Mario Marchionna
Daniele Martella
Luca Mastroianni
Francesco Mauriello
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Francesco Trotta
Alessandro Trovarelli
Rosa Turco
Paolo Vacca
Rosa Vitiello

PL1

Flexible platforms for functional additives in industrial applications

Paolo Vacca*, Stefano Zilio, Miriam Riva, Katarzyna Fidecka, Gabriele Calderoni, Alessandra Colombo

SAES Group Research Labs – SAES Getters S.p.A., viale Italia 77, Lainate

SAES Group Research Labs are continuously engaged in radical research activities to develop new materials and technologies supporting a long-term perspective that continuously puts the company on the edge of innovation. This technology evolution has been also sustaining the SAES growth through different phases until getting a new recent position in fine chemistry area. Many efforts have been devoted during last fifteen years to develop new technology platforms able to create new Chemicals, ranging from functional additives to composite formulations, where sustainability and flexibility are the innovation drivers. The SAES evolution to Chemicals has started from an ancient material like zeolites that SAES has investigated with an innovative approach redesigning the synthetic procedures of this important class of microporous aluminosilicate materials utilizing a green, sol-gel hydrothermal approach. Framed within this context is SAES' development activity, making specialty zeolites suitable for integration of new functionalities in a host of established products. Many different zeolite structures have been developed, encompassing a wide flexibility in terms of pore dimensions, channel geometry and chemical composition. In this paper, we will demonstrate the key features of our zeolites, not only in terms of gas adsorption and biocidal properties, but also according to their environmentally 'green' character, their non-toxicity and safe operation [1-2]. Other innovative platform under continuous development in SAES Labs is related to an innovative membrane based emulsification / nanoprecipitation process, now available on pilot scale. This process is able to sustain the preparation of beads with submicrometric sizes by using polymer materials like EVOH as well as organic materials like polyphenols and ethylcellulose. The opportunity to adopt a new process to transform materials to a spherical form on submicrometric scale is an innovative approach to confer additional features to well known materials overcoming some their intrinsic limitations and strongly widening their application fields [3-4]. The availability of new materials with new shapes and new functions enables the development of innovative products. In SAES Labs innovative additives, i.e. specialty zeolites and beads, are currently adopted to formulate innovative composites suitable to confer active and barrier functionalities in flexible packaging solutions for various applications. Some examples will be presented in terms of functional properties and applications.

Keywords: *zeolites, beads, additives*

* Corresponding author: paolo_vacca@saes-group.com

References

[1] WO2016125050A1 Active package. A. Colombo, M. Riva, P. Vacca.

[2] WO2022101496A1 Antiviral composition comprising modified zeolites. M. Riva, K. Fidecka, P. Vacca

[3] WO2020012396A1 Aqueous ethylene-vinyl alcohol copolymer dispersion and oxygen barrier multilayer film coated with said dispersion. S. Santoro, M. Mudu, P. Vacca

[4] WO2022023503A1 Multilayered flexible package with antioxidant properties, M. Riva, K. Fidecka, P. Vacca

PL2

Sustainability: the Aidic Approach and Engagement

Gaetano Iaquaniello

Associazione Italiana di Ingegneria Chimica

AIDIC has been rethinking the role of the engineer, in particular the chemical engineer, in Society and how to build a bridge between scientific and professional knowledge, and public opinion. Indeed, today there is a strong need to reshape the industry, the industrial processes, and the energy mix into a green and low carbon economy. How can our association have a role into the sustainability contest and help in fighting climate change? How can contribute in defining energy transition targets, technologies and new feedstocks to be adopted, and to introduce or reintroduce wastes into production cycles to develop new models and circularity processes? How to define detailed implementation plans and implement their execution, balancing risks and impacts in the short and long term without jeopardizing the livelihoods and aspirations of a growing global population and maintaining the standards of living in Europe? The AIDIC's commitment to sustainability issues and performance is reflected in the activities of our several working groups, open to external contributors, aiming at developing a shared approach and drafting a position paper on specific subjects related to sustainability from a rigorous Chemical Engineering point of view. Carbon capture and sequestration, decarbonization of the steel industry, hydrogen and mobility, methanol as fuel, and new approaches in agriculture are some of the subjects analyzed. This work highlighted that issues relevant to sustainability are characterized by high levels of complexity and uncertainty, furthermore sustainability goals appear ambivalent in terms conflicts of interests and of values. Since communication plays a crucial role in any sustainability strategy and becomes essential for creating a common understanding on which sustainability's values to work on and concrete goals are required to be implemented, such papers become a key element in a communication campaign strategy aimed at involving public opinion, students, professional people, decision makers through round tables, summer schools, events at universities and on other platforms to discuss in simple, direct, and transparent way all the relevant information on the specific topics. Effectiveness of such a mode of communication about the issues of sustainability is still under review, but in a couple of cases we had a positive interaction with local authorities that allow us to explain and promote our analysis. As far as informing and educating people a clear result was achieved, although it is not easy to assess if recipients have understood the message and changed their values and behaviors. Two examples of such position papers will be illustrated.

Keywords: Sustainability, position paper, communication strategy

g.iaquaniello@nextchem.it

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PL3

Topology and Dispersity: Additional Parameters Regulating the Properties of Bioinert and Functional Polymer Interfaces

Edmondo M. Benetti

Laboratory for Macromolecular and Organic Chemistry (MOC), Department of Chemical Sciences, University of Padova, Padova, Italy

In addition to polymer composition, molar mass, and surface coverage, also the architecture (or topology) and the dispersity of polymer adsorbates represent accessible tuning parameters for modulating the interfacial characteristics of polymer brushes.

When cyclic polymers are applied in the functionalization of macroscopic, inorganic surfaces they generate polymer brushes with enhanced steric stabilization of the interface and a superlubricious behavior, surpassing the attractive characteristics provided by commonly applied, linear polymer brushes [1-3].

The steric and conformational constraints introduced during cyclization additionally affect the characteristics of cyclic polymer assemblies when these feature a functional character. This is the case for polymer interfaces that are chemically designed to actively interact with proteins present in the medium, or, alternatively, which respond to a chemical stimulus by a significant change in their properties [4-5].

Besides the architecture of polymer adsorbates forming brushes, their dispersity appears to be a major factor in controlling different interfacial, physicochemical properties. This is revealed in the case of brushes comprising a poly(methacrylate) backbone and oligomeric side segments, which are broadly employed in materials science and nanotechnology, and feature a structure reminiscent of a large array of biomacromolecules.

A variation in dispersity within polymer brushes regulates the occurrence of hydrophobic, van der Waals interactions between grafts, in turn determining technologically relevant characteristics, such as hydration, adhesive character, lubrication and biopassivity [6].

edmondo.benetti@unipd.it

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MEDAGLIA CHIUSOLI

Unraveling the nature and the identity of the active site in heterogeneous catalysis by a structure-dependent multi-scale and multi-technique approach

Matteo Maestri[1]

1 – Politecnico di Milano, Laboratorio di Catalisi e Processi Catalitici, Dipartimento di Energia, via La Masa 34, 20156, Milano, Italy

There is no doubt that the rational interpretation of the structure-activity relationship in catalysis is a crucial task in the quest of engineering the chemical transformation at the molecular level. In this respect, multiscale analysis based on structure-dependent microkinetic modelling is acknowledged to be the essential key-tool to achieve a detailed mechanistic understanding of the catalyst functionality in reaction conditions[1]. In this talk, I will present the development of a methodology for the study of the structure-activity relationship in heterogeneous catalysis via a structure-dependent multiscale and multi-technique approach. This includes the combined application of both experimental analysis (kinetic experiments, operando spectroscopy) and first-principles and multiscale simulations. Selected examples in the context of CO_2 hydrogenation on metal catalysts and NO oxidation will be used as show-cases[2-5]. As a whole, this methodology makes it possible to reach a molecular level description of the catalyst material in reaction conditions and its catalytic consequences in terms of reactivity. As such, it paves the way towards the use of a rigorous theoretical description for the interpretation of the experimental evidence in terms of structure-activity relationships.

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MEDAGLIA GIACOMO LEVI

Development of Novel Materials for Exhaust Gas Catalysis

Alessandro Trovarelli*[1], Amod Sagar*[2]

1 – Dipartimento Politecnico and INSTM, Università di Udine, via del Cotonifico 108, 33100 Udine - Italy

2 – Treibacher Industrie AG, Department of Catalysis, Auer-von-Welsbach-Straße 1, 9330 Althofen - Austria

Selective catalytic reduction (SCR) is one of the most favored technologies for NOx removal from exhaust of diesel and lean-burn engines. It is widely employed in stationary applications and heavy-duty mobile sources. Among the state of art SCR catalysts, V_2O_5 supported on $TiO_2/WO_3/(SiO_2)$ and Cu or Fe Zeolites are the most widespread and active. Nevertheless, all of these show disadvantages in the application undergoing deactivation during thermal (V_2O_5 supported) and hydrothermal treatments (Zeolites): in addition V_2O_5 based formulations represent an environmental concern due to possible release of V_2O_5 and its toxicity. Here, we describe a new class of modified Fe vanadates (Treibacher's AUERNOX®) that are shown to be valid substitutes of V_2O_5 in SCR catalyst providing i) good activity in at various temperature windows ii) high temperature stability up to 850°C, with no major associated activity loss, iii) absence of toxicological and environmental concern [1,2]. These SCR materials are designed for the production of highly active V-based SCR coatings or impregnations on diverse substrates and are available in several forms including powders, granulates and ready-to-use suspensions. In combination with industrial filters, AUERNOX® can significantly reduce capital expenditures compared to competing solutions, relying on separate DeNOx and oxidation technologies. In addition to SCR, materials based on orthovanadates have been investigated as catalysts for the oxidation of carbon particulate matter [3]. Treibacher and University of Udine are also developing materials *e.g.* high surface area Ceria and Perovskites for CO and soot oxidation.

Keywords: *SCR, soot combustion, oxidation catalysts*

* Corresponding authors: alessandro.trovarelli@uniud.it, Amod.Sagar@treibacher.com

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PREMIO MIGLIOR TESI DI DOTTORATO 2022

Polymer-based Graphene Oxide Derivatives as tunable multipurpose platforms

Angelo Nicosia [1*], Placido Mineo [1]

1 - University of Catania, Polymer Laboratory, Department of Chemical Sciences, Viale A. Doria, 6; 95125 Catania

This communication shows the fundamental role of the polymers in tuning the Graphene Oxide (GO) features, taking full advantage of its structural potentialities. In particular, different polymer-based GO derivatives were designed to obtain advanced nanomaterials having on-demand functionalities for specific applications in sensing, catalysis, and antibacterial coatings: i) a fluorescent sensor for water cationic pollutants was obtained by a noncovalent synthesis between GO and a PEGylated porphyrin derivative. The obtained supramolecular probe shows a turn-on fluorescence ability in presence of paraquat. ii) aiming to perform photocatalytic water remediation, a novel covalent adduct composed of a Porphyrin derivative (used as a light-harvesting moiety) and reduced-GO (used as an electron acceptor), was developed. The resulting nanosystem was embedded, by an in-situ polymerization, in a PMMA substrate. This system was used in form of thin film to perform photocatalytic degradation experiments of pollutants, exploiting solar radiation as an energy source. iii) the antibacterial property is an advanced feature of biomedical devices and common-use objects, usually ensured by low-weight organic molecules used as antimicrobial agents. To overcome the related health issues that have emerged worldwide, a nanotechnological GO-based approach was proposed. Thus, a novel NanoHybrid Graphene, Polymer, and Silver nanoparticles system (NanoHy-GPS) was synthesized through a straightforward microwave-assisted synthetic approach, free of reductants and surfactants. As a proof-of-concept, a preliminary qualitative assay was performed to assess the antibacterial properties of NanoHy-GPS against the typical bacterial population present on common hand-contacted surfaces, demonstrating a significant reduction in the spread of bacterial colonies.

Keywords: *graphene oxide, polymers, photocatalysis, sensors, coatings*

* Corresponding author: Angelo Nicosia, angelo.nicosia@unict.it

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O1

Low Carbon Concrete Admixtures - LCCAs

Giorgio Ferrari[1]

1 - Mapei S.p.A. – Via Cafiero 22 – 20158 Milano

Every year 10 billion cubic meter of concrete are produced. The great success of this material is due to its outstanding properties. In the fresh state, it is castable in formworks of different shapes and size, whilst once hardened it is characterized by its own shape and volume and excellent mechanical properties and durability. These characteristics, together with the large availability and cheapness of the raw materials contributed to make this material so successful. However, such large utilization raised the problem of depletion of the natural resources for its production. Every inhabitant of the planet has an annual "budget" of about 1.25 m3 (1.6 yd3) of concrete, corresponding to about 400 kg (881 lb) cement, 1000 kg (2204 lb) sand and 1200 kg (2645 lb) aggregates. Moreover, about 0.8 kg (1.76 lb) CO2 are produced for every kg (2.2 lb) of cement. This means that, on the global scale, CO2 emissions from cement production count for about 3.2 GTonnes/year, 8 per cent of the total CO2 of human origin. The objectives of improving the sustainability of concrete and limiting the global warming within 2 Celsius compared with the pre-industrial levels by 2100 (2DS scenario) are mandatory challenges for construction industry.
One of the most effective ways to reduce the impact of concrete is to partially replace clinker with supplementary cementitious materials (SCMs) and/or fillers in the cement. New admixtures are needed to improve the performances of concrete with low clinker content (LCC, Low Carbon Concrete). Low Carbon Concrete Admixtures LCCAs can be defined as "concrete admixtures capable of maximizing the performances of blended cements with low clinker content by promoting all the reactions of their constituents capable to contribute to mechanical strength (both early and final strength) without adverse effects on durability".
In this presentation the fundamental mechanisms and performances of LCCAs are presented.

Keywords: *Admixtures, Concrete, Sustainability.*

* Corresponding author: g.ferrari@mapei.it

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O2

Photoresponsive polymers for smart adhesives and surfaces

Martella Daniele[1,2*], Ruggero Rossi[2], Salvini Antonella[3], Parmeggiani Camilla[2,3]

1 - Istituto Nazionale di Ricerca Metrologica (INRiM), Strada delle Cacce 91, Torino
2 - European Laboratory for Non Linear Spectroscopy, via N. Carrara 1, Sesto F.no
3 - University of Florence, Department of Chemistry "Ugo Schiff", Via Lastruccia 3-13, Sesto F.no

Introduction of molecular switches in polymeric architectures is one of the main strategy to obtain intelligent materials, whose properties can adapt to the environment or can be controlled ad-hoc by external stimuli. In this field, azobenzenes are the most commonly used photoresponsive molecules which exploit a *trans-cis* isomerization controlled by selective irradiation. [1] Their introduction in polymeric systems has been described for a wide range of application spanning from artificial muscles activated by light, dynamic optical devices and photopharmacology. In this communication, some examples of photoresponsive polymers based on azobezene or their analogues will be shown focusing on their synthesis and application to obtain smart materials. In particular, polymeric azoetheroarenes have been recently studied as adhesives demonstrating as both the polymeric backbone and the chromophore unit play a crucial role on determining adhesion strength up to a value of 2.8 MPa. By irradiation with UV, the adhesion failed and joint can be detached. On the other hand, addition of a fluorinated moieties on the chromophore has been studied to prepare surfaces whose wettability can be switched from hydrophilic to superhydrophobic under light irradiation. These materials will be explored for the preparation of self-cleaning coating to be applied on different materials.

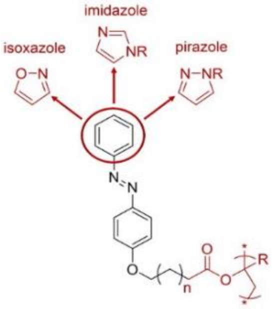

Figure 1 – Structure of photoresponsive polymers based on azoetheroarenes

Keywords: *smart materials, photoresponsive adhesives, photoswitches, acrylic polymers*

* Corresponding author: martella@lens.unifi.it

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O3

Luminescent Solar Concentrators with Outstanding Optical Properties: Cell-Casting and Scaling-Up

Andrea Pucci [1,3*], Alberto Picchi [1], Francesco Ventura [1], Irene Bettini [2], Massimo Ilarioni [2], Massimo Calamante [3], Alessandro Mordini [3]

1 – Department of Chemistry and Industrial Chemistry, University of Pisa, Via G. Moruzzi 13, 56124 Pisa, Italy
2 - I&S srl, Via F.lli Chiaruffi, 12 50067 Rignano sull'Arno, Firenze
3 - Institute of Chemistry of Organometallic Compounds (CNR-ICCOM), Via Madonna del Piano 10, 50019 Sesto Fiorentino, Italy

Luminescent solar concentrators (LSCs) are devices designed to efficiently collect both direct and diffuse solar radiation and concentrate it on photovoltaic cells to foster their use in the building-integrated photovoltaics (BIPV). The optimization of LSCs performances involves the adjustment of both the fluorophore and the guest polymer matrix. On this account, a recently investigated high performance donor-acceptor-donor (D-A-D) photostable fluorophore (DQ1) based on quinoxalinic acceptor core and triarylamines or phenothiazine as donor groups was tested in 5 x 5 cm^2 LSC slabs prepared by cell-casting with 3 mm of thickness. The remarkable optical performances in terms of internal (η_{int}), external (η_{ext}) photon and device efficiencies were compared with those gathered from LSC slabs containing Lumogen Red 305, i.e., the state-of-the-art fluorophore for solar collectors, so far. After assessing the best parameters in terms of DQ1 content to maximize LSC performances, scaling-up procedures were designed to prepare solar collectors with size of 25 x 25 cm^2 and 50 x 50 cm^2 and the same thickness. Final characterization of the large LSC were performed with the aim to assemble them in a photovoltaic bus shelter in Livorno.

Keywords: *solar energy, building-integrated photovoltaics, luminescent solar concentrators, cell-casting,*

* Corresponding author: Andrea Pucci, andrea.pucci@unipi.it

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O4

Conceptual design of a process for the use of liquid ammonia as hydrogen vector

Ilenia Rossetti [1*], Antonio Tripodi [1], Gianguido Ramis [2]

1 - Chemical Plants and Industrial Chemistry Group, Dip. Chimica, Università degli Studi di Milano, CNR-SCITEC and INSTM Unit Milano-Università, via C. Golgi 19, 20133 Milan, Italy
2 - Dip. Ing. Chimica, Civile ed Ambientale, Università degli Studi di Genova and INSTM Unit Genova, via all'Opera Pia 15A, 16145 Genoa, Italy

Chemical energy storage presents a unique feature: flexibility. Chemicals can be moved, stored, and distributed easily, with many of them having a mature market already standing for over decades. Ammonia has been recently presented as a zero-carbon molecule that can provide the required energy storage medium for renewable sources. It can be stored under easy conditions (i.e., refrigerated at −33 °C at atmospheric pressure or at 0.8−1.0 MPa under atmospheric temperature), thus making it a versatile, easy to store medium. Moreover, liquid ammonia has a greater volumetric hydrogen density than liquid hydrogen itself (i.e., liquid hydrogen at 20 K has approximately 70 kg of H_2/m^3, while liquid ammonia at 300 K and 1.0 MPa has 106 kg of H_2/m^3), so that the immediate implementation of an "ammonia economy" can support the futuristic "hydrogen economy". In this work we present the simulation of a plant for the exploitation of renewable hydrogen with production of renewable ammonia as hydrogen vector and energy storage medium. The simulation and sizing of all unit operations were performed with Aspen Plus® as software. Vegetable biomass is used as raw material for hydrogen production, more specifically pine sawdust. The hydrogen production process is based on a gasification reactor at high temperature (700-800 °C), in the presence of a gasifying agent such as air or steam. At the outlet, a solid residue (ash) and a gas, which mainly contains H_2, CH_4, CO and some impurities (e.g. sulphur or chlorine compounds) are obtained. After the removal of the sulphur compounds through an absorption column with MEA (to avoid poisononing of the catalytic processes), 3 reactors are arranged in series: Methane Steam Reforming (MSR), High temperature Water-Gas Shift (HT-WGS), Low temperature Water-Gas Shift (LT-WGS). All the oxygenated compounds must be carefully eliminated: the remaining traces of CO are methanated while CO_2 is removed by a basic scrubbing with MEA (35 wt%) inside an absorption column. The Haber-Bosch synthesis of ammonia was carried out at 200 bar and in a temperature range between 300 and 400 °C, using two catalysts: Fe (wustite) and Ru/C. In conclusion, from an hourly flow rate of 1000 kg of dry biomass and 600 kg of nitrogen, 550 kg of NH_3 98.8 wt% were obtained, demonstrating the proof of concept of this newly designed process for the production of hydrogen from renewable waste biomass and its transformation into a liquid hydrogen vector to be easily transported and stored. The design of a small scale ammonia cracker is also added to demonstrate an integrated process for H2 centralised production and storage and supply to delocalized units.

Keywords: *Ammonia synthesis; Ammonia cracking; Hydrogen storage*

* Corresponding author: ilenia.rossetti@unimi.it

O5

New industrial processes with low environmental impact in the energy and electrodeposition sectors

M. Innocenti [1,2,3*], W. Giurlani [1,2], M. Bonechi [1], A. Comparini [1], M. Verrucchi [1,2].

1 - Department of Chemistry, University of Florence, Via della Lastruccia 3, 50019 Sesto Fiorentino (FI) Italy.
2 - National Interuniversity Consortium of Materials Science and Technology (INSTM), Via G. Giusti 9, 50121 Firenze (FI), Italy
3 - Center for Colloid and Surface Science (CSGI), Via della Lastruccia 3, 50019 Sesto F.no (FI), Italy

The global environmental concerns and the escalating demand for energy, coupled with a steady progress in renewable energy technologies, are opening up new opportunities for the utilization of renewable energy resources. Electrodeposition of semiconducting materials represents a new challenge, not only from the academic point of view, but also from the economic point of view, since this method presents interesting characteristics for large area, low cost and generally low temperature and soft processing of materials. In the field of fuel cells, we aimed at reducing the quantity of catalytic material in order to meet the industrial demand for alternative catalysts be used in place of Platinum-group metals [1]. Furthermore, we developed and characterized new catalyst for fuel cells, based on automotive tires recycling [2]. In the same way galvanic electrodeposition accounts today for almost 40% of the global market value share with North America and Western Europe leading the scenery. Alloy plating offers better answers in terms of economic growth and environmental sustainability due to fine tuning composition, morphology and crystallinity [3]. Here, current trends on alloy electrodeposition research are reviewed highlighting open challenges and process innovations from an industrial perspective. The main categories of alloy compounds are presented and the most important properties for the manufacturing process discussed. Particular attention is devoted to advances in industrial quality control and viable solutions for the reduction of precious metal content in electroplated accessories as well as replacement of cyanide and nickel baths with non-toxic compounds.

Keywords: *Electrodeposition, Energy, Electroplating*

* Corresponding author: Massimo Innocenti: e-mail m.innocenti@unifi.it

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O6

Hazard and operability (HAZOP) application in a Fischer-Tropsch laboratory scale

Grainca A.[1*], Basiri. Z[1], Galli F.[2], Pirola C.[1]

1-Università degli Studi di Milano, Dipartimento di Chimica, Milano (Italy)
2-Universitè de Sherbrooke, Dérpartement de génie chimique (Canada)

Major accidents not only lead to losses of life and capitals, but also cause irreversible damages to the environment.

HAZard and OPerability (HAZOP) study is one of the most widely used and accepted techniques to assess the risk of a process and identify the required safeguards. At the laboratory scale, due to budget and lack of a proper training, often the HAZOP study is neglected, and major hazards are present at the start up and shutdown of the setup. In this paper, the integration of mathematical modelling with the HAZOP analysis, called quantitative dynamic HAZOP study, is investigated for a laboratory scale plant to provide quantitative analysis that define the risks and relative impact of each occurring upset.

The case study reported here refers to a Fischer-Tropsch bench-scale unit (figure 1) where dangerous operating conditions (high pressures and temperatures) and hazardous chemicals (H2, CO, CO2) are involved.

The development of the study concerns an initial conventional HAZOP-analysis, applied for identifying the potential fault causes of abnormal circumstances in the plant.

The second part is devoted to the quantitative HAZOP analysis developed by considering different leakage flows before and after the catalytic bed. The results obtained will be compared with existing data regarding safety measures, as LEL (lower explosion limit) or UEL (upper explosion limit), to define the possible health implication and hazardous level of the plant.

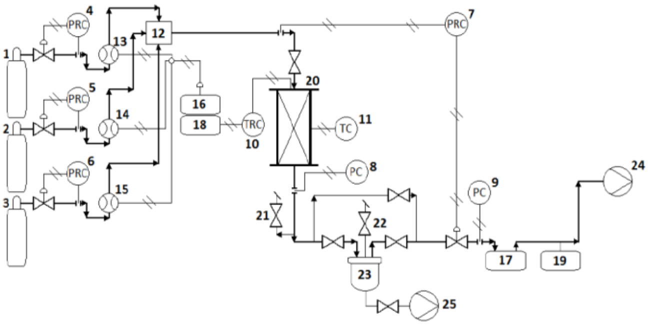

Figure 1 :Fischer-Tropsch laboratory plant

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* Corresponding author: Arian Grainca, arian.grainca@unimi.it

O7

Microwave pyrolysis of waste plastics An overview of the activities at the University of Florence

Luca Rosi

Department of Chemistry "Ugo Schiff", University of Florence, Via della Lastruccia, 3-13, 50019 Sesto Fiorentino, Italy
Renewable Energy Consortium for R&D (RE-CORD), Viale J. F. Kennedy, 182, 50038 Scarperia e San Piero, Italy

The valorization of some waste plastics by thermochemical processes based on Microwave Assisted Pyrolysis (MAP) has been studied in the last decade at the Department of Chemistry of the University of Florence.

Heating a polymeric material is quite complex because heat transfer from the source to the material is usually poor.

Direct MW heating of the material allows, in presence of a suitable susceptor, undoubted process advantages such as rapid heat transfer, fast reaction and adjustable conditions.

Polyolefins, polystyrene, halogenated plastics and some composite materials such as scrap tires and multilayer mixed materials were subjected to MAP optimizing the effect of different operating parameters such as MW power, starting material residence time and recycling of volatiles.

Valuable molecules and, more in general, low-viscosity oils with high heating values were usually obtained, especially when a fractionation system was inserted directly between the furnace and the condensation system.

Presented here are some examples of the pyrolysis studies, as well as the main collaborations with national and international research groups, the available reactor technology at the present and the future perspectives.

Keywords: Microwave pyrolysis; Waste plastics conversion; Fuels from Microwave Pyrolysis of waste, Tires

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O8

Clays as catalysts in biodiesel production from waste lipids

M. Casiello[1]*, S. Savino[1], D. Dinunno[1], M. Massaro[2], A. Monopoli[1], L. D'accolti[1], C. Fusco[3], S. Riela[2], A. Nacci[1]

1 – Università degli Studi di Bari "Aldo Moro", Dipartimento di Chimica, via Orabona 4, 70125 Bari, Italy
2 - Università degli Studi di Palermo, Dipartimento STEBICEF, Sez. Chimica, Viale delle Scienze, Ed. 17, Palermo, 90128, Italy
3 -CNR-ICCOM-SS Bari, Via Orabona 4, Bari, 70125, Italy

The problems related to natural sources depletion, the global climate crisis, and the gradual transition from the linear to the circular economic model, are increasingly pushing the scientific community towards the valorization of wastes and their reintegration into the production cycle. In this context, special attention is attracting exploitation of waste biomass for making energy, in particular to produce biofuels, a process representing an economic and sustainable way for reducing the dependency from fossil fuels and minimizing the greenhouse effect. Among the biofuels, fatty acids methyl esters (FAMEs), namely biodiesel, are ideal and readily usable substitutes of petro-diesel since they can be utilized almost without any engine modification. In the last years, a huge number of papers has been devoted to this topic and a plethora of catalyst systems has been described[1]. With this aim several clays, either in the pristine state or properly functionalized, were screened as suitable catalysts for biodiesel[2] (FAMEs) production from waste lipids. Among them, halloysites and hectorites proved to be the most efficient for the widest range of lipid matrices, among which those extracted from urban wastewater treatment and used cooking oils (WCO). In particular hectorites proved to be more suitable for the transesterification of triglycerides, while nanotubular halloysites, properly modified on their surface, showed to be very active in the direct esterification of free fatty acids (FFA), that commonly compose the waste lipids coming from wastewater treatment. This communication deals with our recent advances in catalytic conversion of waste lipids into FAMEs promoted by clays.

Keywords: *Circular Economy, Biofuels, Clays.*

* Corresponding author: michele.casiello@uniba.it

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O9

Photocatalytic and photoelectrocatalytic H_2 prduction by furfuryl alcohol reforming

Marianna Bellardita*, Claudio M. Pecoraro, Vittorio Loddo, Danilo Virtù, Francesco Di Franco, Monica Santamaria, Leonardo Palmisano

Engineering Department, University of Palermo, Viale delle Scienze Building 6, 90128, Palermo, Italy.

In the last decades, there has been a growing interest in renewable energy sources, due both to the almost exhaustion of the fossil fuels currently used, and to the growth of environmental pollution [1]. The reforming of renewable biomass into fuels and high value chemicals is an ideal and sustainable alternative to the use of fossil resources [2], for instance furfuryl alcohol (FA) can be upgraded to valuable compounds as furfural [3].In this work the photocatalytic (PC) and photoelectrocatalytic (PEC) reforming of furfuryl alcohol (FA), a derivative of biomass, in water solution and ambient conditions was investigated. Both H_2 evolution and partial oxidation to furfuraldehyde were followed. Regarding the heterogeneous photocatalysis, for the first time TiO_2 based photocatalysts were studied for furfuraldehyde and H_2 production and the photocatalytic activity of home prepared photocatalysts was compared with that of commercial ones. In particular, various TiO_2-based catalysts containing different crystalline phases were prepared. Photocatalytic runs were carried out under both UVA and simulated solar irradiation and the influence of metals species presence (Pt, Cu, W, Nb) and pH on the photocatalytic activity and product selectivity were investigated investigated with the aim to improve the performance of bare TiO_2. Photoelectrocatalytic tests were performed by using home prepared TiO_2 nanotubes (TiO_2 NTs) as photoanode and Ni foam as cathode in order to improve the Hydrogen Evolution Reaction (HER). Both the partial FA oxidation reaction rate and H_2 evolution rate were normalized for the lamp specific power to account for the different photon flux and the rates were higher for PEC process. Notably, the materials employed at the anode (TiO_2 NTs) and at the cathode (Ni foam) are Pt free and, they can be used for a large number of tests keeping their activity, being chemically and physically stable in the reaction environment. For these reasons PEC is a promising strategy for the valorization of biomasses with simultaneous H_2 production in spite of the cost of the bias.

Keywords: *Furfuryl alcohol partial oxidation, H_2 production, Photocatalysis, Photoelectrocatalysis*

* Corresponding author: Marianna Bellardita, marianna.bellardita@unipa.it

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O10

Graphene oxide modifications applied on photocatalysis

Stefano Andrea Balsamo [1]*, Roberto Fiorenza [1], Salvatore Sciré [1],

1 – Università degli studi di Catania, dipartimento di scienze chimiche, Viale Andrea Doria 6, 95125 Catania

In the last years, the photocatalysis has been considered one of the best technologies for environmental and energetic applications, thanks to the green utilization of natural or artificial light as driving force for chemical reactions. Water remediation and hydrogen production are two of the most pressing topics in this field. The more common material in photocatalysis is the titanium dioxide, but the performance under the solar light must be improved. Amongst the strategies to enhance the photocatalytic activity, the employing of carbonaceous materials seems to be promising thanks also to a great advantage given by their great adsorbent properties that can help the photocatalysis by proximity effect [1]. Between the carbon-based materials, the graphene in these years kept attention thanks to its peculiar properties such as high conductivity and visible light absorption that make it capable to extend the charge separation lifetime and absorb the solar radiation. In order to avoid the stacking into graphitic structure, often it is used the graphene oxide that is then treated in order to obtain a reduced graphene oxide (rGO) [2]. Here we report a method for a one-pot solar photo-reduction for the GO by the titanium dioxide, in presence of an alcohol as solvent, obtaining a versatile hybrid material [3]. In particular, this peculiar method allows us to obtain satisfying results without using high temperature or hard condition for chemical treatment, as typically carried out for the GO reduction. The obtained samples were tested on water remediation degrading a persistent pesticide (the 2,4 dichlorofenoxyacetic acid) and in the hydrogen production through glycerol photoreforming, reaching good results also compared to other systems more expensive in literature. The materials were investigated in terms of rGO content, reduction degree and irradiation employed for the reductive treatment. To achieve this characterization, were used UV-DRS, FTIR, Raman, XPS, SEM and TEM images and finally BET surface area.

Keywords: *Graphene oxide, Photocatalysis, TiO_2, Hydrogen, water remediation.*

* Corresponding author: Stefano Andrea Balsamo, stefano.balsamo@phd.unict.it

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O11

Development of perovskite-based materials for the photo-catalytic valorization of CO_2

Giulia Forghieri[1], Irene Martin[1], E. Ghedini[1], F. Menegazzo[1], Michela Signoretto[1*]

1 - CatMat lab, Department of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice and Consortium INSTM UdR VE, via Torino 155, Venice 30172, Italy

Carbon capture and usage (CCU) technologies are amongst the alternative strategies aiming to buffer the environmental threaten posed by the increasing amounts of CO_2 in the atmosphere. Although highly desirable, CO_2 conversion is still costly – also due to the required energetic input – and therefore not yet industrially feasible [1]. Photocatalysis involves the use of light as energy source to enable a redox reaction via electronic excitation and, in this context, it could enable CO_2 conversion without additional energy and pollution. However, low selectivity and yields still prevent its industrial application [2]. Therefore, different strategies aiming to improve efficiency, selectivity and photo-responsiveness are meant to enable the diffusion of this catalytic practice. Alkaline-earth-metal-based perovskites have recently emerged as versatile photocatalysts, owed to the possibility to tune both their structure and stoichiometry [3]. Moreover, the intrinsic basicity of alkaline-earth-metal-based perovskites could favour CO_2 adsorption, thereby potentially improving the overall selectivity towards C-based products. In this work, two different types of $BaTiO_3$ perovskites were synthesized via hydrothermal synthesis and tested for the photo-conversion of CO_2 into valuable products. The prepared materials were tested in different reaction conditions to modulate selectivity and yields. While BaTiO3 showed comparable yields to the TiO_2 benchmark, the introduction of CuO NPs to obtain CuO-$BaTiO_3$ and CuO-TiO_2 achieved an increased productivity by both improving selectivity and reducing recombination. This study enabled the development of novel perovskite photocatalyst and the identification of the optimal reaction conditions to maximize selectivity and the photocatalytic performance.

Keywords: *photo-reduction, p-n junction, perovskites, CO_2*

* Corresponding author: miky@unive.it

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O12

Photo-thermo-catalytic H_2 production over flame made $Pt/CeO_2/TiO_2$

Simone Livolsi, Elena Selli, Gian Luca Chiarello*

Università degli Studi di Milano, Dipartimento di Chimica, via Golgi 19, 20132 Milano, Italy

Photocatalytic processes are considered to be temperature independent and are usually operated at room temperature. However, the surface reaction mechanisms can be greatly influenced by temperature. Thus, in this work we have explored the effect of temperature on the photo-steam reforming of methanol ($CH_3OH + H_2O \rightarrow CO_2 + 3 H_2$) over one-step flame made TiO_2, Pt/TiO_2 and $Pt/CeO_2/TiO_2$ photocatalysts. The effect of temperature has been investigated in the range 40-350°C with a home-made stainless steel photoreactor irradiated with a 300 W Xe arc lamp [1]. The presence of Pt nanoparticles (0.75% weight) led to an impressive increase of hydrogen production rate (r_{H_2}), up to ca. 420 mmol h^{-1} g_{cat}^{-1} at 350°C, together with a strong activity also in the dark at temperatures higher than 190°C (Fig. 1). However, in these conditions, the high r_{H_2} is obtained with a high selectivity to CO, as main methanol oxidation product. The selectivity to CO_2 (S_{CO_2}) has been increased from 5% to 55% at 190°C, together with a higher r_{H_2}, upon CeO_2 addition in catalyst formulation (50% weight), due to the Water Gas Shift (WGS) reaction ($CO + H_2O \rightarrow CO_2 + H_2$) promoted by ceria. The effect of temperature on the reaction mechanism under irradiation was studied by operando Modulated Excitation DRIFT (Diffuse Reflectance Infrared Fourier Transform) analysis [2], performed by alternating light and dark condition at different temperature, by in-situ monitoring the dynamics of reactive surface species, including water (3600-3000 cm-1 range), CO_2, CO adsorbed on Pt and formates. This work demonstrated that both r_{H_2} and selectivity to each methanol oxidation products are affected by the operating temperature. Moreover, r_{H_2} and S_{CO_2} can be further increased by the addition of CeO_2. The use of photoreactors combined with solar concentrators may allow the exploitation of powerful synergistic effects between photocatalytic and thermal reactions.

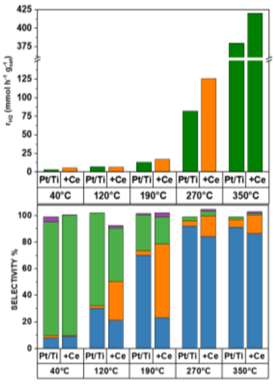

Figure 1 – Hydrogen production rate and selectivity to each methanol oxidation products (blue CO, orange CO_2, green H_2CO and purple HCO_2H) in light conditions at different temperatures for Pt/TiO_2 (Pt/Ti) and $Pt/CeO_2/TiO_2$ (+Ce).

Keywords: *photothermocatalysis, H_2 production, solar fuels, DRIFT*

*Corresponding author: Gian Luca Chiarello, gianluca.chiarello@unimi.it

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O13

Smart Solar products from red vine leaves: an example of how research and the territory can promote a green economy

Elena Ghedini[1*], Lilia Longo[1], Federica Menegazzo[1], Michela Signoretto[1], Alessandro Di Michele[2], Cinzia Pagano[3]

1 – Department of Molecular Science and Nanosystems, University Ca' Foscari Venice and INSTM RUVe, Via Torino 155-30172 Venice
2- Department of Physics and Geology, University of Perugia, Via Pascoli, 06123 Perugia, Italy
3 - Department of Pharmaceutical Sciences, University of Perugia, Via del Liceo 1 - 06123 Perugia.

The potential of agri-food biomass as a raw material for the production of chemicals and fuels has now been widely established and fits perfectly with the paradigms of the circular economy. However, it is today more than ever essential to develop processes that are sustainable at 360 °. This involves the use of local biomass, abundant and easily available, the optimization of energy saving processes and the exploitation of all the components of the biomass avoiding the production of waste. Among the wine waste, red vine leaves, widely present throughout the Italian territory, represent a rich source of secondary metabolites (polyphenols and vitamins) [1] that can be used in a wide range of application from the field of health (dermo-cosmetics, pharmaceutic applications) to the formulation of innovative materials. In this abstract we propose an example related to the use of local red vine leaves (*Vitis vinifera rubra leaf*) for the preparation of Hi-Tech solar products through a 360 ° upgrade process. The phyto complexes deriving from the biomass were obtained through the use of energy saving microwave and ultrasound assisted extraction approaches that allowed to obtain good yields, an optimal composition of the extracts (molecular composition and antioxidant power), by minimizing time and environmental impact of the overall process. The extracts have been used as capping agents for the formulation of ZnO nanoparticles (ZnO NPs). ZnO NPs have been used both as UVA and UVB filters and as stabilizing agents in the formulation of a solar emulsion. Our research shows how the combination of technology, research and territory are among the fundamental prerequisites for using biomass or waste in an efficient and sustainable perspective.

Keywords: *biomass, Red vine leaves, ZnO NPs, UV filter*

* Corresponding author: Elena Ghedini, gelena@unive.it

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O14

Innovative floating photocatalysts for wastewater remediation: a fascinating world merging environmental protection and circular economy

Melissa G. Galloni[1,2*], **Ermelinda Falletta**[1,2], **Elena Ferrara**[1], **Veronica Bortolotto**[1], **Claudia L. Bianchi**[1,2]

1 – Università degli Studi di Milano, Dipartimento di Chimica, Via C. Golgi 19, Milano, 20133, Milano, Italia.
2 – Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali (INSTM), Via Giusti 9, Firenze, 50121, Italia.

Water crisis caused by insufficient water supply and pollution currently leads to several problems related to drought, famine, and death.[1] The treatment of wastewater contaminated by different pollutants is thus of crucial environmental and commercial importance and it urgently requires fast and efficient solutions. Heterogeneous photocatalysis has emerged as an interesting strategy, operating under mild conditions, and degrading many pollutants without chemical oxidant addition.[2,3] In particular, photocatalytic floating devices are currently object of study to overcome issues related to the use of catalyst-based slurry systems and to maximize light utilization, and photocatalyst aeration.[4]

Herein, we present our recent results in the frame of the development and optimization of innovative floating photocatalysts obtained by immobilizing different catalysts (e.g., titanium dioxide, bismuth oxyhalides) on floating supports characterized by eco-friendly features (e.g., alginates, luffa, Lightweight Expanded Clay Aggregate, LECA). A critical insight on the potentialities and/or shortcomings related to each single device will be discussed. A targeted physico-chemical characterization and a proper evaluation of the photocatalytic performances of the obtained devices towards different classes of pollutants (i.e., dyes, drugs, polyphenols) after exposure to solar light irradiation will be described.

The encouraging obtained results deserve a deeper study, but already open the view towards the future use of these systems in real applications, particularly in the perspective of conjugating environmental protection and circular economy.

Keywords: *floating photocatalysts, water remediation, environmental protection.*

* Corresponding author: melissa.galloni@unimi.it

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O15

ZnO@Au Core-Shell Nanoparticles as Efficient Photocatalysts for Photocatalytic Oxidation of VOCs in Air Purification

Luca Spitaleri [1,2]*, Roberto Fiorenza [1], Salvatore Scirè [1], Antonino Gulino [1,2]

1 - University of Catania, Department of Chemical Sciences, V.le Andrea Doria 6, 95125 Catania, Italy
2 - INSTM of Catania, V.le Andrea Doria 6, 95125 Catania, Italy

One of the main problems derived from the recent anthropogenic activity is air pollution caused by the emission of toxic Volatile Organic Compounds (VOCs).[1] Several methods (including adsorption, thermal incineration, catalytic oxidation, etc.) have been proposed to recovery or remove toxic VOCs, but each of these has practical limitations due to the large variety and concentration of different VOCs and process conditions. In this context, the photocatalytic oxidation represents a green, sustainable, and promising method to remove VOCs from air working under milder condition, using renewable energy and some semiconducting materials that are effective in complete mineralizing organic compounds into H_2O and CO_2. ZnO has rarely been studied for the solar photocatalytic elimination of VOCs because it exhibits a high rate of electron-hole recombination and its wide-bandgap makes it promising for ultraviolet detection but less efficient for sun-driven applications.[2] For these reasons, in the present study, we reported the excellent photocatalytic performance and stability of some semiconducting ZnO@Au core-shell nanostructures prepared by a one-pot synthesis towards the gas-phase photooxidation of some common toxic VOCs (toluene, ethanol and formaldehyde) under solar light irradiation. These peculiar nanoparticles show an order of magnitude larger UV-vis photodetection in water solution, number of adsorbed photons, reaction rate and quantum efficiency compared to pure ZnO, due to the additional presence of the surface plasmon resonance of the Au nanoparticles.[3] This photocatalytic behaviour is driven by the efficient electronic communication between the gold core and the zinc oxide shell of these nanostructures, which allows to enhance the overall photodetection of the solar irradiation and improving also the charge carriers separation. In addition, the strong interaction between the ZnO shell and the Au core allowed also to improve the photostability of this nanomaterial, preventing the gold agglomeration and favouring the total oxidation of the VOCs. Therefore, ZnO@Au nanostructures can be considering promising candidates as an efficient photocatalyst for air purification.

Keywords: *ZnO@Au, core-shell, photocatalytic oxidation, VOC*

* Corresponding author: Luca Spitaleri, luca.spitaleri@phd.unict.it

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O16

Well-Defined Polymers via Aqueous Emulsion Atom Transfer Radical Polymerization

Francesca Lorandi [1*], Marco Fantin [1], Yi Wang [2], Krzysztof Matyjaszewski [2]

1 – University of Padova, Department of Chemical Sciences, via Marzolo 1, 35131, Padova, Italy
2 – Carnegie Mellon University, Department of Chemistry, 4400 Fifth Avenue, Pittsburgh, Pennsylvania, 15213, USA

Aqueous emulsion polymerizations are industrially relevant processes because of their environmentally friendly character, facile heat transfer, and absence of volatile organic compounds. In *ab initio* emulsion polymerizations, radicals are generated in the aqueous phase, then particles are nucleated, stabilized by surfactant molecules, and continuously replenished by monomer molecules diffusing from big monomer reservoirs. Such biphasic systems pose a challenge if a catalyst needs to be introduced to control the propagation of radical chains.

Atom transfer radical polymerization (ATRP) is a well-established technique to prepare polymer materials with pre-determined molecular weight (MW) and architecture. The implementation of ATRP in emulsion is limited by the need to design a catalyst capable of initiating radicals in the aqueous phase and then regulate the polymerization occurring inside growing hydrophobic particles. The simple combination of an hydrophilic commercial catalyst (a complex of $CuBr_2$ with tris(2-pyridylmethyl)amine) and the anionic surfactant sodium dodecyl sulfate (SDS) was found to effectively control emulsion ATRP via both interfacial and ion-pair catalysis.[1,2,3] Well-defined homopolymers and copolymers were obtained with part per million level of the Cu complex, by introducing a water-soluble reducing agent or by using light irradiation.[3,4] The surfactant loading could be reduced to < 3 wt%, and the latexes showed long-term stability.

Keywords: *emulsion polymerizations, ATRP, well-defined polymers*

* Corresponding author: Francesca Lorandi, francesca.lorandi@unipd.it

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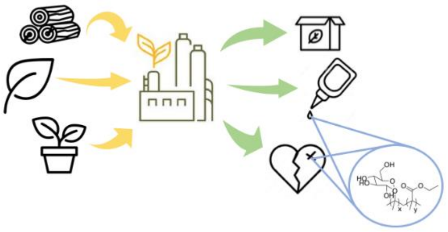
O17

Biopolymers from biomass valorization towards new functional materials

Alice Cappitti [1*], Camilla Parmeggiani [1], Antonella Salvini [1]

1 – University of Florence, Department of Chemistry "Ugo Schiff", Via della Lastruccia 3-13, 50019 Sesto Fiorentino

Smart materials, able to perform actions under stimulation, are receiving increasing interest in the biomedical field. However, besides the requirement to fit the biological and mechanical properties of the investigated tissue, also the attention towards the environment needs to be addressed and their preparation calls for technological solutions with reduced environmental impact. In this scenario, the use of biopolymers has therefore increased considerably. with applications in the most various fields, from medical to packaging, from adhesives to the conservation of cultural heritage. In order to obtain polymeric formulations with high performances, the monomers must be selected appropriately to obtain specific structure with chemical-physical characteristics modulated for each application field [1]. In this research several saccharides have been used as starting material to produce innovative biopolymers with a structure containing polar and reactive groups capable of influencing the application behavior. In particular α,α'-trehalose and α-D-glucose were used as feedstock in order to obtain new monomers for the following copolymerization. The synthetic methodology involved the functionalization of α,α'-trehalose and α-D-glucose through different reactions. In particular substitution and transesterification reactions were used in order to introduce polymerizable groups, such as allyl and acrylic groups. Such monomers were used for the synthesis of both, vinyl acetate and ethyl methacrylate copolymers, always through radical copolymerization reactions. These biopolymers have been performed in accordance with the requirements of low environmental impact and will be evaluated for the preparation of artificial muscles, new adhesive formulations or in the field of cultural heritage.



* Corresponding author: alice.cappitti@unifi.it

Keywords: *biopolymers, saccharides, biomass valorization*

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O18

Cryogels platform for the removal of emerging pollutants

Sandro Dattilo [1*], Chiara Zagni [2] Tommaso Mecca[3], Andrea A. Scamporrino[1], Roberta Puglisi[1], Sabrina Carola Carroccio[1*].

[1] *Institute for Polymers, Composites, and Biomaterials CNR-IPCB, Via Paolo Gaifami 18, 95126, Catania, Italy*
[2] *Department of Drug and Health Sciences, University of Catania, V.le A. Doria, 95125, Catania, Italy*
[3] *Institute for Biomolecular Chemistry CNR-ICB, Via Paolo Gaifami 18, 95126, Catania, Italy.*

A platform of polymeric cryogels based on methacrylic acid (C-mA) meglumine (C-megl), lysine (C-lys), and 2-hydroxy ethyl methacrylate (C-ph), as well as a combination thereof having both negatively and positively charged moieties, have been synthesized and used to capture emerging contaminants from water[1]. Their specific properties in sequestering antibiotics (Levofloxacin, Ampicillin, Doxycycline), anti-inflammatory (Piroxicam), antifungal (Fluconazole), anti-parasite (Moxidectin), pesticides (2,4D) and dyes (Thymol blue, Methylene Violet) were tested considering their ionic charge in solution. The adsorption experiments performed in batches at different pH and pollutant concentrations have demonstrated the outstanding ability of these macroporous sponges in complexing molecules by the instauration of different type of interaction, also in the presence of inorganic ionic species such as arseniate. In addition, it was demonstrated as the novel dual-material, that have opposite ionic charge cryogels can simultaneously remove antagonist dyes. Almost total release of the target molecules was achieved by variation of pH, allowing the regeneration of the sponges for multiple re-uses maintaining its performance[1]. The latter peculiar feature may be adopted for drug delivery applications since the release can be modulated and programmed by a specific pH modification.

Keywords: *cryogel, polymer, emerging pollutant, antibiotic, dye, 2,4 D, adsorption, drug delivery.*

* Corresponding author: sandro.dattilo@cnr.it

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O19

Improved sustainability of thermosetting polyurethanes with Design of Experiment

Gabriele Viada [1], Nicole Mariotti [1], Simone Galliano [1,2*], Alberto Menozzi [3], Federica Tammaro [3], Walter Gianelli [3], Matteo Bonomo [1], Claudia Barolo [1]

1 - University of Torino, Department of Chemistry, NIS Interdepartmental Center and INSTM Reference Centre, Via Pietro Giuria 7, 10125 - Torino, Italy
2 - University of Torino, Department of Agricultural, Forest and Food Sciences, Largo Paolo Braccini 2, 10095 – Grugliasco (TO), Italy
3 - Demak Polymers, Strada del Cascinotto 163, 10156 – Torino, Italy

In recent years, the use of polyurethanes (PUs) has enormously increased in the industrial context thanks to their versatile synthesis and tunable physicochemical properties. Nowadays PU-based materials are massively used in many fields, from building construction to automotive, until biomedical application.[1] However, PUs present some critical issues not completely solved yet. Above all, the massive use of fossil-based components as well as the extensive use of mercury-based catalysts, that is now significantly restricted by European legislation, still raise evident environmental concerns. It is therefore essential to implement alternative reagents and catalysts, aiming to improve the sustainability of polyurethanes while reducing resource consumption and carbon footprint.[2,3]. In this contribution, made in collaboration with Demak Polymers company, the formulation of a commercial polyurethane resin for LED encapsulation has been investigated in order to implement bio-based and recycled components and to remove toxic catalyst, while maintaining optimal characteristics in terms of optical transparency, UV light and thermal stability. To proceed in the most economical and efficient way possible, the Design of Experiment (DoE) approach was successfully applied for this investigation. The DoE is a multivariate statistical method allowing to simultaneously evaluate the influence of different factors on the selected responses, giving information on the whole experimental domain. The DoE analyses allowed to identify an optimal PU formulation with greatly improved sustainability while ensuring satisfactory specifications for commercial purpose.

Keywords: *polyurethane, sustainability, design of experiments*

* Corresponding author: simone.galliano@unito.it

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O20

Influence of the addition of plastic waste residues in coal blends for coke production

Massimo Bernardini [1*], Marcello Pagliero [1], Gustavo Capannelli [1], Paolo Petit Bon [2], Giancarlo Bruni [3], Antonio Comite [1]

1 Dipartimento di Chimica e Chimica Industriale & UdR INSTM, Università degli Studi di Genova, via Dodecaneso, 31, 16146 Genoa, Italy
2 Ireos Laboratori S.r.l., via Stefano Turr, 165, 16147 Genoa, Italy
3 Italiana Coke S.r.l, via Stalingrado, 25, 17014 Cairo Montenotte (SV), Italy

Nowadays, non-recyclable plastic waste can be disposed of by combustion in waste-to-energy plants or used after processing as a secondary solid fuel (SSF) additive for the production of cement. The addition of polymers to the coal blends used for the production of coke is also a very interesting alternative that can enhance its use while effectively limiting the emission of CO_2 into the atmosphere. Several studies have focused on the quality and quantity of plastic to be added to the feed mixture as well as the quality of the coke obtained in the pyrolysis process. It has been found that SSFs containing mainly polyolefins are preferable [1] and that the amount of plastic should not exceed 5% (w/w). This improves the mechanical properties of the coke. The introduction of this type of materials in the coke oven process must be carefully considered due to their high volatility, which can cause overpressure problems [2]. On the other hand, the increase in coke oven gas (COG) production can have positive effects thanks to the possibility of further exploitation, such as the production of electricity or the production of syngas. In this study, the influence of adding small amounts of non-recyclable plastic waste to coking coal blends was examined. Initially, the effect on coke quality was tested in a pilot plant, using coal blends for foundry coke and steel coke production. Afterwards, the influence of plastic content on gaseous and condensable products was evaluated by performing coking processes in a laboratory-scale plant. The coal blends containing up to 5% (w/w) were heated to 800 °C in an inert atmosphere. During the process, the gas produced was analysed using a micro-gaschromatograph (μ-GC) to quantify H_2, CH_4, C_2H_6, ethene C_2H_4, CO, and CO_2, while tar and waxy products were identified and quantified with a gaschromatograph-mass spectrometer (GC-MS). It was observed an improvement in cold mechanical strength for foundry coke using SSF as coal feed additive, due to a more compact coke structure, while mechanical properties of steelmaking coke, despite a slight deterioration, remained acceptable. However, it was also found that using coking coal mixture with high acidity index for steelmaking coke, coke strength increased. As for the COG, the yields obtained confirmed a higher formation of gas by increasing the amount of plastic in the blend, while the yield of condensable products was mainly influenced by the type of coal. For foundry coke, the higher production of gas was largely related to an increase of H_2, while for steelmaking coke the formation of every gas was greater. The results obtained from the GC-MS analysis performed on the condensable products showed that the presence of plastic reduced the formation of 3 and 4-ring polycyclic aromatic hydrocarbons and phenol and its derivates, while an increase in naphthalene and linear hydrocarbons was observed. In conclusion, the use of SSF in the coking process is beneficial since a better-quality coke is produced and the dispersion of nanoparticles in the environment is reduced due to the higher compactness of the final product. Furthermore, and not less significant, the new process implementing the use of SSF to integrate the coal blend avoids the direct combustion of the waste plastic material, and in turn the emission of CO_2 in the atmosphere, producing a more valuable COG richer in H_2. The support of P.O.R. FESR LIGURIA 2014-2020–Asse 1 "Ricerca ed Innovazione" is acknowledged.

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O21

Photosensitized Thermoplastic Nano-Photocatalyst for Potential Applications in Extraterrestrial Facilities

Lidia Mezzina[1,*], Angelo Nicosia[1], and Placido Giuseppe Mineo[1]

1- Department of Chemical Sciences, University of Catania, V.le A. Doria 6, Catania, Italy;

Nowadays space colonization is one of the most popular topics, leading many space agencies to launch several space missions. However, considering that future space missions (such as NASA's Artemis Program) have the goal of settling humans on the Moon (and later on Mars) the presence of xenobiotic pollutants in closed environments could represent a health risk for organisms exposed to long-time exposure in a close environment. Indeed, the scarceness of primary resources such as air and water and the importance of their purification and recycling have determined the need to seek new low-energy depollution methods. Photocatalysis activated by solar light is a promising depollution method that uses reactive oxygen species (ROS) to mineralize organic pollutants. One of the most used photocatalysts is titanium dioxide in form of nanoparticles (TiO_2 NPs) [1]. However, the photocatalytic approach is unsuitable to be used in underground facilities and/or space environments (e.g., extraterrestrial facilities), because the photocatalytic mechanism of TiO_2 cannot be promoted by photons generated from the indoor lighting system, since they don't have enough energy to activate the photocatalysts [2]. Finally, recovery of the photocatalytic slurry from the depolluted solution is not easily feasible, particularly in low-gravity conditions. To overcome the above issues, we produced different filmable nanocomposites using the in-situ radical copolymerization of an ad-hoc synthesized porphyrinic macromonomer (the photosensitizer) and methyl methacrylate directly into TiO_2 NPs. This approach aims to improve the photocatalytic performance of TiO_2 by ensuring intimate contact between the photocatalyst and the photosensitizer, also exploiting the PMMA waveguide effect [3]. The photocatalytic activity of the so-obtained nanocomposites was verified against both common dye probes and recalcitrant xenobiotic pollutants, employing light sources falling in the visible light range (λ>390 nm). The experimental data showed that the sensitized nanocomposites' photocatalytic performance is about double that of the unsensitized nanocomposite. This improved effect is due to the photosensitizer which could act both as an electron transfer and/or a dopant agent, boosting the TiO_2 photocatalytic efficiency. Thanks to their intrinsic properties (good filmability, thermal stability, wettability, etc), this new kind of thermoplastic nano-photocatalyst is suitable to be used in the form of thin films as an auxiliary system to the already employed depolluting systems in unconventional sceneries: underground or Low Earth Orbit laboratories, or (potentially) in future lunar shelters [4].

Keywords: *Photocatalysis, Porphyrin, Copolyacrilates, Space Facilities*

* Corresponding author: Lidia Mezzina, lidia.mezzina@phd.unict.it

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O22

3D printed light-activated polymer

Matteo Gastaldi[1], Francesca Frascella[2], Marco Zanetti[1,3], Andrea Fin[1], Silvia Bordiga[1], Claudia Barolo[1,3], Ignazio Roppolo[2]

1 Department of Chemistry and NIS Interdepartmental Centre and INSTM Reference Centre, University of Torino, Via Pietro Giuria 7, 10125 Torino, Italy
2 Department of Applied Science and Technology, Politecnico di Torino, C.so Duca degli Abruzzi 24, 10129, Turin, Italy
3 ICxT Interdepartmental Center, University of Turin, Lungo Dora Siena 100, 10153 Torino, Italy

Dyes play a crucial role in everyday life, and recently they have been exploited to confer innovative functionalities to polymers. Among others, organic light emitting diodes (OLEDs), liquid crystals (LC), displays and optical data storage represent some innovative uses of organic molecules.[1] Usually, these dyes can express their peculiar functionality under external stimuli, such as light, pH, solvent or temperature, producing stimuli-responsive polymeric devices. On the other side, further innovations can be observed in the production techniques, among which additive manufacturing (AM), also called 3D printing (3DP), is transforming the manufacturing field by achieving both complex and functional structures that cannot be fabricated by other means. 3DP relies on vat photopolymerization, such as digital light processing (DLP), which has gained much attention due to its superior print resolution, relatively high speed, low cost, and flexibility in the material.[2] Combining the stimuli-responsive polymers and the DLP 3D printing technique, we can obtain 3D printed high-complex structures, incorporating the 4th dimension into 3D printed static polymers. In particular, in this work, we produced a formulation containing a very low quantity of azodyes dissolved in a photopolymerizable monomer that can be 3D printed using a DLP configuration printer. The resulting polymer can increase its temperature under 532 nm green laser irradiation in a very huge and rapid manner. The temperature can rapidly increase from room temperature to more than 100°C in a very localized area: only the part containing azodyes can be heated, while the blank parts remain unchanged. Thanks to this phenomenon, we can modify the elastic modulus of the resulting polymers through a reversible process that does not produce thermal or photo degradations. This peculiar property can be useful to activate sensors remotely or to induce shape-memory recovery.

Keywords: *azodyes, 3D printing, DLP, photopolymerization*

* Corresponding author: Ignazio Roppolo, ignazio.roppolo@polito.it

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O23

The case of study of hazelnut shells biorefinery: Synthesis of active carbons from the hydrochar recovered downstream of levulinic acid production

Domenico Licursi [1*], Claudia Antonetti [1], Nicola Di Fidio [1], Sara Fulignati [1], Patricia Benito [2], Monica Puccini [3], Sandra Vitolo [3], Anna Maria Raspolli Galletti [1]

1 - University of Pisa, Department of Chemistry and Industrial Chemistry, Via G. Moruzzi 13, 56124, Pisa, Italy
2 - Dipartimento di Chimica Industriale "Toso Montanari", Alma Mater Studiorum – Università di Bologna, Viale Risorgimento 4, 40136, Bologna, Italy
3 - Department of Civil and Industrial Engineering, University of Pisa, Largo Lucio Lazzarino, 56122, Pisa, Italy

Hazelnut processing industry generates significant waste streams, in particular cuticles and shells. Extractives are the main components of the cuticle fraction (~36 wt%), mainly including polyphenols and fatty acids, which can be advantageously employed in the pharmaceutical and cosmetic industry. Focusing on the shell fraction, this represents ~50 % of the total nut weight. Differently from cuticles, shells are rich in recalcitrant lignin (~38 wt%), in addition to cellulose and hemicellulose (each component accounting for ~23 wt%). Up to now, this waste, which is preponderantly produced in Italy and Turkey, is mostly underutilized, being limitedly used as a boiler fuel for domestic heating and for landscaping. On the other hand, both these fractions of hazelnut shells can be successfully valorized and, in agreement with the objectives of the project PRIN 2020 LEVANTE "LEvulinic acid Valorization through Advanced Novel Technologies" (2020CZCJN7), we have proposed a new cascade approach, converting its cellulosic fraction into levulinic acid (~9-12 wt%), recovering as final waste an abundant carbonaceous hydrochar (~45 wt%), mainly composed of aromatic (from lignin) and furanic (from degradation of C5/C6 sugars) units. In the LEVANTE project, this hydrochar was activated by pyrolysis and chemical treatments (H_3PO_4, $ZnCl_2$, KOH, NaOH), and the synthesized new active carbons (ACs) have been properly characterized (ultimate and proximate analysis, FT-IR, surface properties and SEM microscopy). This preliminary screening allowed us to select the KOH-AC as the most interesting one, as further confirmed by the highest CO_2 adsorption capacity (~90 mg/g), due to its well-developed microporous texture. This new AC was also effective for the removal of the bulkier methylene blue (complete removal, corresponding to ~250 mg/g). This proposed integrated approach makes possible to fully exploit the hazelnut shell feedstock, smartly closing the biorefinery cycle of the hazelnut wastes, in a circular economy perspective. In addition, the selective fractionation of soluble C5 and C6 sugars of shell fraction is currently under investigation and this will enable us to obtain an hydrochar with a less-degraded lignin fraction, thus moving towards progressively more sustainable hydrothermal and activation reaction conditions.

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Keywords: *hazelnut shells, levulinic acid, hydrochar, active carbons*

* Corresponding author: Domenico Licursi, domenico.licursi@unipi.it

O24

Kinetics of Levulinic acid esterification with ethanol: from batch to continuous operation

Francesco Taddeo [1*], Carmelina Rossano [1], Martino Di Serio [1], Vincenzo Russo [1]

1 – University of Naples Federico II, Chemical Sciences Department, Via Cintia I-80126 Naples, Italy

Levulinic acid is considered one of the most important chemicals as it is a versatile building block for a variety of high value-added products that can be involved in a wide range of applications. Catalytic esterification of levulinic acid with alkyl alcohols leads to levulinate esters to be used as fragrances, flavoring agents and fuel additives [1,2]. Esterification reactions are usually performed in the presence of both homogeneous and heterogenous catalysts. The main disadvantages of using homogeneous catalysts are the corrosion of the reactors, separation and reusability of the catalyst itself, the purity of the products and the presence of side reactions [3]. Some of these problems can be solved by replacing homogeneous catalysts with heterogeneous solid acid catalysts. Among them, heteropoly acids, zeolites and ion exchange have been tested. The main benefits connected with their use is their reusability, they are non-corrosive and easily recovered [2,3]. Levulinate esters, such as ethyl levulinate are extremely interesting thanks to their properties as they find applications as specialty chemicals, in petrochemical industries, as fuel additives, flavors, in the polymers synthesis and an attractive alternative is their use as precursor for the ketals synthesis [1,4]. Levulinate esters can be produced from the reaction between levulinic acid and various types of alcohols. In this work, the esterification of levulinic acid with ethanol in the presence of Amberlite IR120 as heterogeneous catalyst was studied, and a detailed kinetic investigation was made. In particular, tests were firstly performed in a batch reactor varying different operative conditions (i.e. stirring rate, temperature, catalyst loading and alcohol:acid molar ratio) and the collected experimental data were interpreted with a reliable kinetic model considering the occurrence of the intraparticle mass transfer limitation. In order to validate the obtained results, experiments were also conducted in a fixed bed reactor and in this case a fluid-solid limited kinetic model was developed to simulate the experimental data.

Keywords: *Biomass, levulinic acid, esterification, kinetics*

* Corresponding author: Francesco Taddeo, francesco.taddeo@unina.it

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O25

Development of cellulose-based materials for rigid packaging applications

Francesco Prandi [1*], Daniele Caretti [1], Giovanni Mazzotti [2]

1 - Dipartimento di Chimica Industriale "Toso Montanari", Viale del Risorgimento 4, 40136, Bologna
2 - SACMI Imola S.C., Via Selice Provinciale 17/a, 40026 Imola

Cellulose is the most abundant renewable biopolymer that exists in natural resources and has been used as material for packaging and other applications owing to its peculiar features such as biodegradability, low cost, light-weight, and easy recyclability. However, cellulose cannot be processed by conventional technologies (such as extrusion) and is a hydrophilic matrix that tends to strongly interact with water.

Therefore, the development of cellulose-based rigid packaging designed for contact with food and beverages is not simple and requires very thorough study. With the goal of producing hydrophobic and recyclable cellulose-based packaging, both the technological aspects of cellulose dry molding and the characteristics of the material to be molded were investigated. A dry molding process offers several advantages (including primarily high productivity) over wet molding processes, that are commonly used for cellulose processing. Molding tests were carried out using molds of different sizes to produce disc-shaped specimens. These tests allowed to investigate the relation between the characteristics of the raw material and the properties of the molded object. In addition, the best process conditions, such as mold temperature, pressure applied to the object, and cycle time, were found by such preliminary tests. For pressure up to about 250 bar, there is generally an increase in density of molded samples as temperature and applied pressure increase. Moreover, materials consisting of shorter fibers generally achieve higher density by compression molding. At the same density value, the greater the length of the cellulose fibers, the greater the resistance of the material under bending tests [1]. When a pressure of 1,000 bar or more is applied to the object, the upper density limit of cellulose is reached, and no significant change in density and mechanical properties is observed as process conditions change. In order to produce a hydrophobic sample suitable for food and beverage applications, it is not sufficient to use a highly compacted cellulose sample. In fact, although the kinetics of water absorption is greatly affected by the compaction level achieved [2], even samples molded at very high pressure absorb a significant amount of water. Therefore, the last phase of the project involved the synthesis of several sizing agents commonly used in the paper industry for cellulose hydrophobization [3]. Compression molding of cellulose fibers blended with different weight percentages of the various synthesized sizing agents resulted in the production of hydrophobic samples (characterization by water contact angle analysis as well as water uptake and sealing tests), suitable for rigid packaging applications.

Keywords: *cellulose, packaging, circular economy*

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O26

Microwave-assisted reductive amination of aldehydes and ketones over Rh-based heterogeneous catalysts

Maela Manzoli[1]*, Fabio Bucciol[1], Emanuela Calcio Gaudino[1], Alberto Villa[2], Maria Carmen Valsania[3] and Giancarlo Cravotto[1]

1 - Università degli Studi di Torino, Dipartimento di Scienza e Tecnologia del Farmaco e Centro Interdipartimentale NIS, Via Pietro Giuria 9, 10125, Torino, Italy.
2 - Università degli Studi di Milano, Dipartimento di Chimica, via Golgi 19, I-20133 Milano, Italy.
3 - Università degli Studi di Torino, Dipartimento di Chimica, Via Pietro Giuria 7, 10125, Torino, Italy.

Amines are essential bioactive compounds in nature, but are also widely used in man-made products such as pharmaceuticals[1,2] and polymers[3,4]. To obtain amines, reductive amination of aldehydes is the most employed approach and it offers different advantages: mild reaction conditions, high atom economy and abundance of substrates to choose from. Ketones are also possible substrates[5], even though generally regarded as less reactive. Herein, microwave (MW)-assisted reductive amination of aldehydes and ketones were carried out in the presence of heterogeneous Rh-based catalysts. Homemade catalysts were prepared using ultrasound (US) to improve the metal dispersion, whereas commercial activated carbon and carbon nanofibers were used as supports. The results were compared with those obtained with supported Rh commercial catalysts to envisage the effect of US. Moreover, different natural-occurring molecules were chosen as substrates for the reaction and aqueous ammonia was used as a cheap and non-toxic reagent. MW coupled with heterogeneous Rh catalysts allowed a mitigation of the reaction parameters[6] allowing a 98.2% yield in benzylamine (starting from benzaldehyde) working at 80 °C with 10 bars of H_2 for 1 h; and a 43.3% yield in phenylethylamine (from acetophenone) working at 80 °C with 5 bars of H_2 for 2 h. Carbon nanofibers were found to be a better support for the metal phase with respect to simple activated carbon since a limited yield in benzylamine (10.6 %), but a high selectivity for the reductive amination of ketones were obtained. In particular, raspberry ketone was converted to raspberry amine with a 63.0 % yield. A screening of different substrates proved that the reaction is easily transposed; notably, ketones were well converted over Rh/C despite literature reporting that aldehydes are the preferred substrates for the reductive amination.

Keywords: *MW-assisted reductive amination, microwave, ultrasound, Rh catalyst*

* Corresponding author: Maela, Manzoli, e-mail contact: maela.manzoli@unito.it

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O27

Role of PVA-based polymeric stabilizers on catalytic activity of gold nanostructured materials

Stefano Scurti[1,2]*, Francesca Liuzzi[1,2], Alessandro Allegri[1,2], Filippo Capancioni [1], Nausica Tacconelli [1], Stefania Albonetti[1,2], Nikolaos Dimitratos[1,2], Daniele Caretti [1,2]

1 – Department of Industrial Chemistry 'Toso Montanari', University of Bologna, Viale Risorgimento 4, 40136 Bologna (Italy)
2- Center for Chemical Catalysis-C3, Alma Mater Studiorum Università di Bologna, Viale Risorgimento 4,40136 Bologna, (Italy)

Recently, a growing numbers of researchers have focused on the role of the polymeric stabilizers employed to prevent colloidal nanoparticles aggregation and coalescence, as tools to tune the properties of the prepared nanomaterials such as their shape and size. As a consequence, also their properties from the catalytic point of view can be modified in terms of conversion, selectivity and availability of active sites.[1-3] In particular, it has been reported that the polymer features like molecular weight, degree of functionalization as well as the presence of specific functional groups on the macromolecular chains can influence the catalytic activity due to a combination of steric and electronic effects. [4-5] In this work has been investigated the influence of PVA-based copolymeric stabilizers with different hydrolysis degree and functional groups in the side chain. In particular PVA-PVAc and PVA-PVAm copolymers have been synthesized and employed as polymeric stabilizers during colloidal gold nanoparticles preparation method. The supported nano-catalysts were tested in model reactions that involved reductions of nitro/azo-aromatic pollutants persistent in the water environment as well as the oxidation of hydroxymethyl furfural (HMF). [6] The chosen reactions have been studied to correlate structure-properties features with the observed catalytic activity in order to rationalize the role of the polymeric stabilizers on the catalytic performances

Keywords: polymeric stabilizers, nanocatalysts, water treatment, HMF

* Corresponding author: Stefano Scurti, stefano.scurti2@unibo.it

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O28

Synthesis of methyl-levulinate catalyzed by an ion-exchange resin: a kinetic investigation

Michele Emanuele Fortunato [1]*, Francesco Taddeo [1], Martino Di Serio [1], Vincenzo Russo[1]

1 – University of Naples Federico II, Department of Chemical Sciences, Via Vicinale Cupa Cintia 26, 80126 Napoli.

The depletion of fossil fuels has pushed towards the use of renewable raw materials. Among these, biomass is widely used. Lignocellulosic biomass is a starting material for obtaining important platform chemicals such as levulinic acid (LA) which has been classified by the United States Department of Energy as one of the best chemical compounds for the synthesis of many value-added products for its versatile chemistry [1]. The esterification of LA with primary alcohols (i.e. methanol, ethanol, etc.) is of great interest since, the derived esters, such as methyl levulinate, find many applications as green solvents, fuel-additives, fragrances component, medical drugs synthesis, plasticizers, etc.[2]. Homogeneous acidic catalysts (e.g. liquid mineral acids like HCl, HNO_3, $H2SO_4$) have been widely used in the esterification reactions because they ensure high yield of esters, but such catalysts suffer from disadvantages such as difficult recovery and product extraction, equipment corrosion and environmental pollution. Therefore, over the past decade, solid acids (e.g. zeolytes, metal oxides, HPAs and ion-exchange resins) have gained broad prospects as efficient heterogeneous catalysts for the esterification of LA given the advantages of environmental friendliness, mild reaction conditions, high yield, selectivity, easy recovery, and reusability. In this regard, resins, due to their high acidity and long-lasting activity, are attractive heterogeneous catalysts to be employed in the synthesis of levulinates. The present work reports the kinetics of the esterification of levulinic acid with methanol catalyzed by DOWEX® 50-WX8, an ion exchange resin produced in the form of thin spherical beads whose gel-type lattice consists of a styrene-divinylbenzene copolymer. Several experiments have been carried out in a batch reactor at different experimental conditions to study the effect of the temperature, the agitation speed, the catalyst bulk density and the LA-to-methanol ratio on the reaction kinetics. A mathematical model has been developed to simulate the behavior of the system, considering also the intraparticle diffusion limitations and the experimental data have been submitted to nonlinear regression analysis to obtain kinetics and thermodynamic parameters. The authors are grateful to Italian Ministero dell'Istruzione dell'Università e della Ricerca for the financial support provided through the LEVANTE project "LEvulinic acid Valorization through Advanced Novel Technologies", Progetti di Ricerca di Rilevante Interesse Nazionale -Bando 2020, Prot. 2020CZCJN7.

Keywords: *levulinic acid; biomass; esterification; kinetics; heterogeneous catalysis.*

* Corresponding author: Michele Emanuele Fortunato, micheleemanuele.fortunato@unina.it

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O29

Acrylic pressure-sensitive adhesives
A "green" chemistry route

Ludovica Di Lorenzo [1*], Simone Bordignon [2], Michele Remo Chierotti [3], Valentina Giovanna Brunella [4]

1 – Department of Chemistry and Nanostructured Interfaces and Surfaces (NIS) Centre, University of Turin, Turin, 10125, Italy

The continuous demand for more sustainability and regulations in constant increase by the world authorities lead to the development of environmentally more suitable alternatives to petroleum-based materials. The adhesive industry, in particular, is looking for more renewable alternatives and more environmentally friendly synthesis routes. In this work, isobornyl methacrylate derivative of terpenoid and geraniol alcohol monoterpene, are introduced in the synthesis of waterborne pressure-sensitive adhesives (PSA) based on acrylic latex via emulsion polymerization. Numerous formulations have been prepared with different but always relevant biobased contents. The adhesives were chemically characterized with Fourier transform infrared (FTIR) spectroscopy, thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), and nuclear magnetic resonance NMR. Many of these formulations show good adhesion proprieties on painted steel, PE, and paperboard surfaces. Formulated PSAs were compared in terms of adhesive strength with an oil-based commercial product. However, the various formulations exhibit different adhesive properties, which can be interesting for a fair range of applications.

Keywords: *Pressure-sensitive adhesives, Acrylic, Sustainability*

* Corresponding author: Ludovica Di Lorenzo, ludovica.dilorenzo@unito.it

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O30

Co-based catalysts for CO_2 hydrogenation: methanation vs. reverse water gas shift activity

E. Spennati [1], P. Riani [2], G. Busca[1], G. Garbarino[1]*

1 - University of Genoa, Department of Civil, Chemical and Environmental Engineering,
Via all' Opera Pia 15, Genoa, Italy
2 - University of Genoa, Department of Chemistry and Industrial Chemistry,
Via Dodecaneso 31, Genoa, Italy

Environmental pollution represents one of the main international concerns nowadays. In this contest, around 31.5 Gt of global energy-related CO_2 emissions were produced in 2021 [1]. A possible strategy to mitigate this environmental problem is the conversion of CO_2 using green hydrogen. Co-based catalysts are active for the hydrogenation reactions and in particular, Co supported over Al_2O_3 is the industrial catalyst for the low-temperature Fisher-Tropsch process using CO [2,3]. In this study, Co-supported catalysts (5 and 13.6 wt.%) over commercial alumina and silica-alumina (5 wt.% silica) were prepared and tested for CO_2 hydrogenation. Co-based catalysts were prepared by wet impregnation and calcined at 1023 K for 5 hours. For the assessment of catalytic performance, the catalysts were pre-reduced in situ with a stream containing 20% v/v of H_2 and 80% v/v of N_2 (flow rate 80 NmL/min). Catalytic experiments were performed in a tubular fixed-bed silica glass reactor, loaded with 88 mg of catalyst and 700 mg silica particles. 80 NmL/min of gaseous reactant mixture, in diluted condition with nitrogen, were fed to the reactor with a GHSV of 55000 h^{-1} and an H_2/CO_2 ratio of 5. The reaction temperature was varied step by step from 523 to 773 K (ascending temperature) and from 773 to 523 K (descending temperature). Fresh and exhausted catalysts were characterized by means of XRD, FE-SEM, FT-IR, and UV-vis-NIR techniques. In general, it was observed that modifying cobalt content the support composition, it is possible to shift the reaction activity from Sabatier to RWGS reaction or vice-versa. The highest RWGS activity was obtained using 5 wt.% of Co supported over alumina (50% of CO yield at 773 K). The 13.6% of Co supported on silica- doped alumina showed the highest activity in methanation reaction producing a maximum methane yield (51% at 723 K).

Keywords: *CO_2 conversion, Co-based catalysts, Synthetic Natural Gas*

* Corresponding author: G. Garbarino, gabriella.garbarino@unige.it.First author: E. Spennati, elena.spennati@edu.unige.it

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O31

Desalination by photothermal membrane distillation

Pagliero Marcello[1,2]*, Comite Antonio[1,2], Costa Camilla[1,2], Rizzardi Ilaria[1], Servida Alberto[1]

1 - Department of Chemistry and Industrial Chemistry, University of Genoa, Via Dodecaneso 31, 16146, Genova, Italy
2 - National Interuniversity Consortium of Materials Science and Technology (INSTM), Florence, Italy

Membrane distillation (MD) is a thermally driven separation process in which a vapor pressure difference at the two sides of hydrophobic porous membrane leads to a net mass flux of water vapor from a hot feed to a cold side. The hydrophobic character of the membrane is a mandatory requirement to prevent liquid leaking and to maintain high retention factors for non-volatile compounds. Thanks to its modular configuration, low power consumption and ability to exploit low grade energy resources, MD has a great potential to become one of the best technologies for the development of off-grid desalination/wastewater treatment plant [1]. To this end, many attempts to design solar MD plants have been carried out, generally coupling traditional solar collectors to simple membrane modules. In the last few years, a new configuration has been proposed: photoactive membrane distillation (PMD). PMD is based on the development of new membranes that are able to convert the solar energy into sensible heat directly on their surface. The heat is then transferred to the feed by conduction, directly in the boundary layer in contact with the membrane surface, reducing – or even reversing – the temperature polarization phenomenon that is normally generated by the water evaporation [2]. In this work the several phases of the development of a small PMD setup are discussed. First, a suitable photoactive mixed matrix membrane was prepared by a simple non-solvent induced phase separation technique including carbon black (CB) inside the starting polymeric dope solution. The concentration of CB and polymer were tuned to obtain a membrane with the desired properties. Several samples were then tested in a lab-scale distillation setup, assessing their distillation performance under controlled light irradiation. Finally, a small PMD pilot setup was developed in order to evaluate the long-term stability of the membrane operating under real conditions. To this end, the membrane was mounted in the cell and the plant was placed under direct sunlight at the Department of Chemistry and Industrial Chemistry of the University of Genoa, Italy. The plant feed was seawater and the main process parameters were continuously monitored as well as the actual incident solar irradiance. Exposing the membrane to solar light increased the feed temperature up to 45°C and induced a distillate flux enhancement of around 100% compared to the tests performed in similar conditions, but covering the membrane from solar light.

Keywords: photothermal membrane distillation, mixed matrix membrane, PVDF, desalination.

* Corresponding author: Marcello Pagliero, marcello.pagliero@unige.it

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O32

Reduction of CO_2 to Methanol on Cu (111): DFT study

Federica De Luca*[1], Salvatore Abate[1], Gabriele Centi[1], Siglinda Perathoner[1]

1 - Department of ChiBioFarAM (Industrial Chemistry), University of Messina, ERIC aisbl and INSTM/CASPE, V.le F. Stagno d'Alcontres 31, Messina 98166, Italy

Theoretical calculations were performed, using density functional theory (DFT), to estimate the Reaction and Activation Energy (E_a) of the elementary steps involved in the hydrogenation of CO_2 to methanol (CO_2+ $3H_2$= H_3COH+H_2O) on the Cu surface.[1] All the calculations were performed using the meta generalized gradient approximation (meta-GGA-MSRPBEL) functional in the Vienna ab initio simulation package (VASP). Cu-based heterogeneous catalyst is one of the most active and promising for selective CO_2 hydrogenation. The pathway via formate (HCOO) intermediates to reduce CO_2 was studied. The elementary steps were performed on a Cu slab about 5x5x10 Å considering the surface with Miller's index (111). To begin, the calculations were performed to determine the most favorable adsorption orientation of reaction intermediates. The calculations highlight that, because of the stability of CO_2, a physisorption occurs on Cu (111) surface. Indeed, an indirect activation of CO_2 need to be performed. It was noted that the gaseous CO_2 can interact with the adsorbed hydrogen and the bond C=O is able to be weakened and therefore dissociated in the intermediates. The formate intermediates species can easily absorbate on Cu (111) surface and were observed to be stable. The geometry optimization of each intermediate and then reactants and products were calculated in order to obtain the reaction energy. Afterwards, Nudges Elastic Band (NEB) and Dimer calculations were performed. The goal is to calculate the saddle point of the potential energy surface in order to find the transitional state of each elementary step.
Nevertheless, the unfavorable interaction between CO_2 and Cu (111) surface, the main reaction (CO_2+H^*=$HCOO^*$) presents a reaction energy equal to -0.36 eV and an activation energy about 0.85 eV. As consequence, in order to produce methanol, via formate pathway, HCOO requires to be subsequently hydrogenated to H_2COOH and then dissociated into H_2CO and OH. This reaction is vital to produce methanol because H_2CO has to be hydrogenated following the elementary step H_2CO^*+H^*=H_3CO^*. The reaction should occur easily thanks to the E_a equal to 0.19 eV. As consequence the last step is the hydrogenation of H_3CO that leads to the methanol production with a reaction energy of 0.11 eV and a E_a about 1.28 eV[2]. Finally, DFT simulation was used to investigate methanol synthesis via CO_2 hydrogenation on Cu (111) and the obtained results highlight that the reaction is able to occur by the formate pathway.

Keywords: *CO_2 hydrogenation, DFT, Cu (111), formate pathway*

* Corresponding author: Federica De Luca, fedeluca@unime.it

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O33

Membrane aeration unit: study of the oxygen mass transfer from air to water

I. Rizzardi[1]*, A. Bottino[1], G. Capannelli[1], C. Costa[1], R. Firpo[1], M. Pagliero[1], A. Comite [1]

1- membrane&membrane Research Group, Department of Chemistry and Industrial Chemistry (DCCI), University of Genoa, Via Dodecaneso 31, 16146, Genova, Italy

The term aeration refers to the operation of transferring oxygen from a gaseous phase to a liquid phase [1]. It accounts for about 60-80% of the total costs of the depuration process due to the high-energy demand associated with the use of compressors. The main issue affecting the process is the low solubility of oxygen in water, which limits the mass transfer at the liquid/gas interface. The mass transfer coefficient K_La is made up of the contribution of the overall volumetric transfer coefficient (K_L) and of the specific available exchange surface area (a). Therefore, to promote the oxygen mass transfer is possible a) improve K_L acting on fluid dynamics or b) increase the gas/liquid interfacial area. Aerators supply oxygen to the system through the generation of bubbles, the total surface area of which represent the useful interface for the mass transfer. Conventional systems, such as perforated disks, have a standard oxygen transfer efficiency (SOTE) of approx. $8.5\%\cdot m^{-1}$ and $9.8\%\cdot m^{-1}$ which corresponds to less than 30% in 3 m high tank. Porous membranes are an interesting alternative as they have a high porosity, which in turns results into a high exchange surface area and a low volume of the equipment. Furthermore, when the membrane is acting in contactor mode between the gas and liquid phase, it can work either without or with bubble formation [2,3]. The bubble-free mode is interesting in application such as membrane aerated biofilm reactors (MABR). In this configuration, the interfacial area is related only to the membrane surface properties. In bubble mode the specific interface is the prevalently due to the overall surface offered by the emitted bubbles. The aim of the work is to study the aeration and in particular the feasibility of membrane systems for the aeration. Several membrane modules were prepared using hollow membrane fibers. Aeration tests were carried out using the sulfite method exploring different operating parameters. K_La and SOTE, were evaluated and compared with that of conventional commercial aeration disks. The membrane module in bubble mode showed a better overall mass transfer efficiency even if the mechanism of bubble formation needs still to be better studied and understood.

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Keywords: aeration, membrane, mass transfer

* Corresponding author: I. Rizzardi 1, ilaria.rizzardi@edu.unige.it

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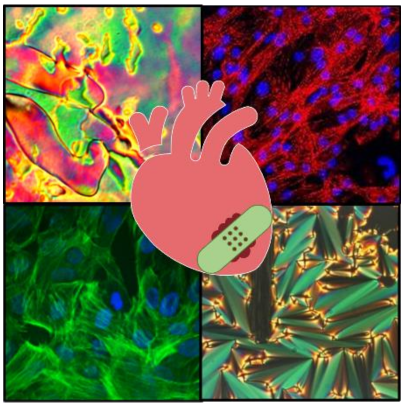
O34

Smart materials based on liquid crystals for tissue engineering

Camilla Parmeggiani [1,2*], Daniele Martella [2,3], Cecilia Ferrantini [2,4], Leornardo Sacconi[2,5], Antonella Salvini[1]

1 – University of Florence, Department of Chemistry, via della Lastruccia 3-13 Sesto F.no
2 – European Laboratory for Non-Linear Spectroscopy (LENS), via N. Carrara 1, Sesto F.no
3 – Istituto Nazionale di Ricerca Metrologica (INRiM), strada delle Cacce 91, Torino
4 - University of Florence, Department of Experimental and Clinical Medicine, Largo Brambilla 3, Firenze
5 – National Research Council, National Institute of Optics, via N. Carrara 1, Sesto F.no

Development of stimuli-responsive polymers is currently a hot topic in many research fields and new synthetic approaches are demanding to obtain the specific properties fitting the needs of each specific application. Among them, Liquid Crystalline Networks (LCNs) are promising candidates to address unsolved tissue engineering issues [1]. In particular, acrylate-based LCNs combine the easy processability with a demonstrated biocompatibility towards different cell lines such as human induced pluripotent stem cell derived cardiomyocytes. Furthermore, the LC alignment inside the materials was demonstrated instructive in myoblast culture and able to promote their differentiation into functional myotubes [2]. On the other hand, advanced materials able to work as actuators for the treatment of muscle injuries, could combine rapid and long-lasting intervention, which is the main goal in muscular regenerative medicine. LCNs could result in a good advancement also in this field since, once stimulated, they can mimic muscle force production [3].



Additionally, the preparation of new monomers deriving from biomasses towards more sustainable LCN preparations and the implementation of the material properties is currently explored.

Keywords: *smart materials, tissue engineering, liquid crystalline networks*

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* Corresponding author: Camilla Parmeggiani, camilla.parmeggiani@unifi.it

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O35

Insights on the recyclability of Sn/HAP materials for reduction of Cr(VI) in semi-real waters

Tiziana Avola [1*], Sebastiano Campisi [1], Ludovica Ferruti [2], Antonella Gervasini [1]

1 - Dipartimento di Chimica, Università degli Studi di Milano, via C. Golgi 19, I-20133 Milano, Italy
2 - A2A S.p.A, Group Risk Management, Enterprise Risk Management, C.so di Porta Vittoria, 4 - 20122 Milano

Among conventional technologies for the removal of toxic hexavalent chromium from industrial wastewaters, reductive adsorption is an alternative promising approach consisting in the combination of two steps: reduction of Cr(VI) and adsorption of the formed Cr(III) ions onto the material surface. In the last years, tin(II)-hydroxyapatite based materials (Sn/HAP) have been developed for this purpose by our research group. Calcium hydroxyapatite ($Ca_{10}(PO_4)_6(OH)_2$) is a cheap eco-friendly material that possesses well established adsorption ability towards several heavy metal ions, according to different mechanisms, such as ion-exchange, surface complexation, dissolution-precipitation.[1] To date, the maximum uptake of chromium from aqueous solutions onto Sn/HAP material[2] has been reported to be up to 20 mg/g. Despite these promising results, there is a lack of information about the recycle possibility and the effect of other co-ions present in aqueous solutions on reductive performances. Co-ions may both influence double-layer at the solid interface and compete towards adsorption sites of Sn/HAP. In this study, tin-functionalized hydroxyapatite with Sn nominal loading of 10 wt% (Sn10/HAP) was prepared and tested in simulated semi-real waters. Tests of Cr(VI) reduction ($[Cr(VI)]^0$ = 20 mg/L) were carried out in batch at 25°C and at acidic pH (~ 2) for 2h. Then, recycle experiments have been carried out making up to seven tests on the same solid material after the separation of the liquid phase. To evaluate the effect of co-ions we have considered the composition of "real" wastewaters, kindly provided by *a2a company* (Ca^{2+}, Mg^{2+}, Na^{+}, Fe^{3+}, Al^{3+}, Zn^{2+}, Mn^{2+}, Cl^{-}, NO_3^{-}, SO_4^{2-} ions in a concentration range 20 - 200 mg/L). Ion Chromatography and Inductively Coupled Plasma Mass Spectrometry (ICP-MS) techniques have been used to determine the residual ion concentration after test, while TEM, XPS and XRD techniques are used to evaluate the metal dispersion on solid surface. First of all, the effect of all the co-ions on the Cr(VI) removal was negligible: removal efficiency of 99.99% is reached in all different ionic media. Moreover, Sn10/HAP showed higher affinity towards trivalent cations (Fe^{3+} and Al^{3+} ions) leading to removal efficiencies up to 98% and 95%, respectively. Conversely, concerning the alkaline and alkaline earth metals, such as Na^{+} and Mg^{2+}, removal capacity lower than 5% is reached. In conclusion, tin-hydroxyapatite based materials showed a good reuse capacity up to the first two cycles, then the removal efficiency gradually decreased in the next cycles. Furthermore, the effect of co-ions is not dramatic and, potentially, Sn/HAP could be used also as efficient material for wastewater remediation in real waters.

Keywords: *hydroxyapatite, Cr(VI) reduction, tin dispersion, recycle*

* Corresponding author: Tiziana Avola, tiziana.avola@unimi.it

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O36

Sonochemical synthesis of iron based nano-hydrotalcites promoted with Cu and K as catalysts for Fischer-Tropsch synthesis in biomass to liquid process

Di Michele A.[1*], Grainca A.[2], Pirola C. [2], Bianchi C. L.[2], Boccalon E.[3], Nocchetti M.[4]

1 - Università di Perugia, Dipartimento di Fisica e Geologia, Perugia (Italy)
2 - Università degli Studi di Milano, Dipartimento di Chimica, Milano (Italy)
3 - Österreichische Akademie der Wissenschaften, Vienna (Austria)
4 - Università di Perugia, Dipartimento di Scienze Farmaceutiche, Perugia (Italy)

Fischer–Tropsch synthesis (FT) is a well-known industrial process able to convert syngas mixture into valuable products as long-chain hydrocarbons. FT can also be applied in the conversion of CO_2/H_2 mixtures, and for this reason, this technology is attracting interest in biomass conversion processes. However, different catalytic materials are required to activate the stable CO_2 molecule than those used in the traditional process. In this study, a series of nano ternary hydrotalcites (HTlcs) were prepared with and without ultrasound to obtain active Fe-based catalysts for the Fischer–Tropsch synthesis. HTlcs can be easily prepared and essentially consist of mixed metal hydroxides, where specific metal atoms are homogeneously dispersed at an atomic level. All the samples in new and used form were characterized by XRPD, ICP-OES, SEM-EDX, TEM, FT-IR, BET, TPR, and TG and tested in a fixed bed reactor. Ternary HTlcs constituted of Mg, Cu and Fe were synthesized both employing an ultrasound-assisted co-precipitation method (MCF_US) and a solvent-free method carried out by ball mill (MCF_BM). FT tests were performed in a fixed bed reactor loaded with 1 g of fresh catalyst.

HTlcs were activated in H_2 or syngas atmosphere and characterized by different techniques: XRD, SEM-EDX, and TEM. Similarly, HTlcs were tested in FT synthesis after different activations, i.e., in H_2 or syngas atmosphere. The CO conversion and the selectivity towards methane, CO_2, light, and heavy hydrocarbons were determined. The CO conversion resulted higher and more stable for syngas-activated catalysts. The selectivity was very low (40%) for higher chain hydrocarbons. The formation of carbide species in syngas activation should explain these results.

Keywords: *Fischer-Tropsch, HTlcs, High Power Ultrasounds, Ball Mill,*

* Corresponding author: alessandro.dimichele@unipg.it

O37

Adsorption kinetic of iopamidol onto activated carbon

R. Paparo[1*], M. Fortunato[1], G. Carotenuto[3], F. Uggeri[2], V. Russo[1], M. Di Serio[1], M. Trifuoggi[1], L. Nicolais[4]

1 - Università degli Studi di Napoli, via Cintia, 4. IT-80126 Napoli,
2 - Bracco SpA, Research & Development Division, Via E. Folli 50, 20134 Milano,
3 - IPCB-CNR, Piazzale E.Fermi, 1. IT-80056 Napoli
4- Materias Srl, Corso N. Protopisani 70, 80146 Naples

Nowadays, a new class of emerging contaminants are pharmaceutical compounds such as X-ray contrast media that are widely used in the modern society [1].
Iodinated X-ray contrast media (ICM), has become the focus of environmental concern because they are highly hydrophilic displaing high aqueous solubility, meaning that they are difficult to eliminate from water and wastewater [2]. Iopamidol ($C_{17}H_{22}I_3N_3O_8$) is a pharmaceutical compound beloging to the class of the non-ionic and monomeric iodinated constrast media. Conventional wastewater treatment processes are uneffective in removing these compounds leading to their appearance in surface water, effluents of wastewater, and groundwater. In this regard, different technologies have been developed for the treatment of wastewater. Adsorption is the best methods, thanks to its great applicability due to low cost, simplicity, and versatility [3]. To study the adsorption kinetics of Iopamidol onto activated carbon a Iopamidol solution (initial concentration 100 mg/L) is mixed with different activated carbon types to find the most efficient one. So, a series of adsorption tests are conducted in a thermostated, stirred glass-jacketed reactor changing the amount of activated carbon (from 1 to 0.01g), temperature, stirring velocity (800,600,400 rpm) to find the best parameters that allow high Iopamidol remotion with lower amount of adsorbent. The activated charcoal samples are characterized before and after adsorption/desorption experiments using thermogravimetric analysis (TGA), differential scanning calorimetry (DSC) and diffusion reflectance infrared Fourier transform (DRIFT) spectroscopy.

Keywords: adsorption, wastewater, iopamidol, activated carbon

* Corresponding author: Rosanna Paparo, rosanna.paparo@unina.it

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P1

Hydrogen and Carbon use through Energy from Renewables

S. Albonetti[1]*, F. Basile[1], A. Allegri[1], A. R. De Angelis[2], R. Millini[2], B. Federico[2], M. Giacinti Baschetti[3], F. Melino[3], V. Cozzani[3]

1 – University of Bologna, Department of Industrial Chemistry, Viale Risorgimento 4, 40136 Bologna
2 – ENI SpA, Research & Technological Innovation Department, Via F. Maritano 26, 20097 San Donato Milanese, Italy
3 – University of Bologna, Department of Civil, Chemical, Environmental, and Materials Engineering (DICAM), Via U. Terracini, 28 - 40131, Bologna
4 – University of Bologna, Industrial Engineering Department (DIN), Viale Risorgimento 2, 40136 Bologna

Hydrogen and CCUS are recognized by the European Commission and in Horizon Europe as transversal themes with high potential to achieve the objectives of the Green Deal and neutrality in climate-changing emissions by 2050. In particular, both technologies are attributed a significant role in the decarbonization of "Hard to Abate" industrial sectors such as chemicals, steel, materials and fertilizers production Furthermore, hydrogen is believed to play a strategic role in obtaining energy carriers to be used in heavy transport and long distance starting from railway and naval ones, both directly (LH) and through derived e-fuels (NH_3, CH_4, liquid fuels). In many of these areas, the use of hydrogen is associated with the capture and use/storage of CO_2 and the production and transformation of renewable energy. The University of Bologna and Eni are developing in Ravenna a Joint Research Laboratory dedicated to Hydrogen and Carbon use through Energy from Renewables. This research lab is centered on three interconnected pillars, in strong partnership with the new investments in the decarbonization sector present in the area:

- Sustainable and safe production and use of hydrogen
- Capture, Use Storage of CO_2 in synergy with the transformation of hydrogen
- Technologies with potentially negative CO_2 emissions

The initiative addresses the creation of a strategic innovation laboratory on the production and use of hydrogen and on the capture and use of CO_2 that accompanies the projects of international importance present on the territory [1-3]. A place to encourage close collaboration between public and private sectors for the development of technologies capable of shortening the time to market of innovative solutions.

Keywords: *H_2 production, CO_2 capture and use, CCUS, mineralization*

* Corresponding author: Stefania Albonetti, stefania.albonetti@unibo.it

P2

Biomass-derived catalysts: synthesis and characterization of hydrochars and pyrochars

C. Antonetti*, D. Licursi, B. Bertini, N. Di Fidio, S. Fulignati, A.M. Raspolli Galletti

University of Pisa, Department of Chemistry and Industrial Chemistry, Via G. Moruzzi 13, 56124, Pisa, Italy

Lignocellulosic biomass is one of the more important renewable sources and it will play a strategic role in many future markets, taking into consideration that a renewable energy share of 32% is binding at the European level by 2030 [1]. Deconstruction of lignocellulosic biomass can be carried out via hydrothermal processes and, among them, hydrothermal carbonization (HTC) represents a versatile process, which promotes the progressively deoxygenation of the biomass, under relatively mild reaction conditions (T up to about 250 °C for 48 h) [2]. This is an environmentally and low-cost treatment, thus resulting suitable for any type of biomass, including wet and waste ones. The obtained solid-rich product, called hydrochar, can be used in a wide range of applications, such as adsorption, energy storage, CO2 sequestration, catalysis etc. In this last field, within the project PRIN 2020 LEVANTE "LEvulinic acid Valorization through Advanced Novel Technologies" (2020CZCJN7), different hydrochars have been synthesized starting from cellulose and the effects of the main reaction parameters, such as reaction time, temperature and substrate loading, have been investigated employing statistical modelling. The adopted central composite design has allowed us to identify the best reaction conditions (220°C for 5h, with 20 wt% of cellulose loading), in order to maximize both the hydrochar yields and its reactive functionalities. For this purpose, the synthesized hydrochars have been characterized by elemental analysis, SEM, EDS, FT-IR, TGA, whereas the recovered liquid phase has been analyzed by HPLC. Under the selected set of processing parameters, the yield of hydrochars was in the range 38-48 wt%, with a carbon content of 60-70 wt% and corresponding higher heating values amounting to 17-27 MJ/kg, confirming the successful conversion of cellulose into a carbonaceous material. Moreover, Boehm titration has been applied to quantify acidic functional groups, in particular carboxylic, lactonic and phenolic ones, whose amounts increase under more severe reaction conditions. For comparison, the best reaction parameters have been also adopted for the synthesis of hydrochars starting from glucose and xylose as reference model compounds. Finally, on the basis of final applications, also pyrochars have been prepared starting from the optimal hydrochars, working at 600°C with a heating rate of 10°C/min, in order to increase the aromatization degree and the surface areas. All the synthesized hydrochars and pyrochars will be further functionalized and employed, as acid catalysts, for the valorization of levulinic acid, in particular for its conversion to diphenolic acid, in agreement with the objectives of the project LEVANTE.

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Keywords: *hydrochars, pyrochars, levulinic acid*

* Corresponding author: Claudia Antonetti, claudia.antonetti@unipi.it

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P3

Application of polymer traditional technology to obtain bio-based materials based on protein/peptide from rapeseed byproducts

Sara Aquilia,[1,2,3] **Sabrina Bianchi**,[3] **Michele Pinna**,[3] **Anna Maria Papini**,[1,2] **Claudia Bello**,[1,2] **Francesco Ciardelli**,[3] **Luca Rosi**[2]

1- Laboratory of Peptide & Protein Chemistry & Biology-PeptLab, University of Florence, I-50019 Sesto Fiorentino, Italy
2- Department of Chemistry "Ugo Schiff", University of Florence, Via della Lastruccia 3-13, 50019 Sesto Fiorentino, Italy
3- Spin-Pet s.r.l., Viale Rinaldo Piaggio, 32 - 56025 Pontedera,Italy

Proteins have recently attracted much attention in the search for new eco-sustainable polymeric materials. Despite their availability and favourable properties that would make them suitable for these applications, proteins present some limitations, such as their slow biodegradability only occurring under composting conditions, scarce mechanical properties, and excessive hydrophilicity[1].

Here we present our preliminary work toward the development of biocompatible and renewable protein-based materials from vegetable sources. In particular, proteins from rapeseed oil co-products[2] have been chosen as first candidates for our bioplastics main ingredient. After characterization and appropriate purification of this proteins, we applied polymer traditional technology and chemical and enzymatic reactions to modulate their thermo-mechanical properties. The obtained bio-based material combines the processability properties typical of petrol-based plastics and the eco-sustainability of the proteins. Selection of other potential sources of proteins, and standardization of the methodology will expand the toolbox for the preparation of advanced versatile biomaterials for packaging.

To develop a fully sustainable bioplastics, we designed and prepared peptides, deriving from appropriately characterized protein lysates. Because of their high compatibility with the proteic matrix, these peptides will be employed as additives in protein-rich materials. The obtained results will contribute to the *green transition* achieving the goals of the *European Green Deal*.

Keywords: *polymeric material; protein; rapeseed by-products; sustainability*

* Corresponding author: Sara Aquilia

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P4

SiC-based photocatalysts for the solar H_2 production by photoreforming of sustainable organic substrates

Maria Teresa Armeli Iapichino[1*], Marta Calà Pizzapilo[1*], Roberto Fiorenza[1], Stefano Andrea Balsamo[1], Salvatore Scirè[1]

1 – University of Catania, Department of Chemical Sciences, Viale A.Doria 6, 95125, Catania (Italy).

The H_2 production by photoreforming of organic substrates is an attractive way to obtain green H_2 together with the valorisation of biomass or waste. Indeed, this reaction can be exploited not only to increase the evolution of this fundamental energy carrier but also to produce high added value compounds from byproducts. For this purpose, the choice of the organic substrate is fundamental to drive selectively the products formation and to enhance the charge carrier separation generated on the surface of the photocatalysts, being the substrates holes scavengers. In this context, the use of molecules derived from biomass as the cellulose, is very promising. To efficiently solubilize the cellulose that is a necessary step for the photoreforming reaction, there are necessary various pre-treatments which hard conditions can easily deactivate the most common photocatalysts. The silicon carbide (SiC) a widely used semiconductor in the electronics industry, can be employed, especially in the last years, as photocatalyst and it is particularly suitable for the photoreforming applications based on renewable substrates. In particular in this work, we have obtained a good H_2 production (900 μmol H_2/g_{cat} ·h) in the cellulose photoreforming at neutral pH, using a 0.5% wt Au/TiO_2-2% wt SiC composite, where the gold was deposited on the physical mixture of commercial SiC and TiO_2 P25 with a solar one-pot photoreduction method [1]. Furthermore, the same SiC with the addition of the 0.5% wt of g-C_3N_4, synthetized with the thermal degradation of urea, gave promising results in the photoreforming of bisphenol A, a common plasticizer, at basic pH (12 μmol H_2/g_{cat} ·h), considering that this photoreforming was a more difficult reaction. The good affinity between the SiC and the carbon nitride, favoured by their structures and chemico-physical features [2] allowed to valorise the plastic waste and to propose fascinating solutions for both energy and environmental problems as the plastics pollution in the water, highlighting also the high versatility of the SiC-based photocatalysts.

Keywords: *H_2 production, silicon carbide, gold, plastics, cellulose*

* Corresponding authors: Maria Teresa Armeli, armeliteresa12@gmail.com; Marta Calà Pizzapilo , marta.cala20@gmail.com

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P5

Effect of the addition of different metal species on TiO_2 photocatalysts used for glucose and fructose reforming

Marianna Bellardita*, Muhammad Umair, Leonardo Palmisano, Vittorio Loddo

Engineering Department, University of Palermo, Viale delle Scienze Building 6, 90128, Palermo, Italy.

Biomass is a green renewable resource easily available and considered a precious alternative to non-renewable sources for the production of valuable chemicals and fuels [1]. Hexoses, such as glucose, or fructose, are among the most abundant monosaccharides present in biomass and their transformation can give rise to a variety of platform chemicals. The catalytic oxidation of these substrates under severe conditions (high temperature and pressure, organic solvents, presence of soluble bases) has been widely investigated. In this context, heterogeneous photocatalysis can be considered as an enviromental friendly and cheap alternative to traditional chemical process [2]. Although different papers report the photocatalytic selective oxidation of glucose and/or fructose in aqueous solution to high value chemicals, no high conversion and selectivity values have been obtained. This work reports the preparation of several TiO_2 based photocatalysts modified with different metal species (Pt, Nb,Cu) with the aim to improve the performance of the system towards both H_2 production and high added value compounds formation. The runs were carried out under anaerobic conditions in aqueous medium and ambient conditions. In the liquid phase the formation of different valuable compounds as arabinose, erythrose, formic acid, fructose and gluconic acid was observed whilst CO_2 and H_2 were measured in the gas phase [3]. Home prepared catalysts displayed higher activity with respect to the commercial TiO_2 samples. Naked TiO_2 was inactive towards H_2 production, copper was effective in replacing Pt, the presence of Nb was beneficial both for H_2 production and selective oxidation. The results obtained with the same catalysts were slightly different with the two substrates highlighting the importance of the powder surface-organic compound interaction. The highest hydrogen amount was ca. 360 μmol g^{-1} h^{-1} in the presence of Nb.

Keywords: *TiO_2 photocatalysts, glucose, fructose, H_2 production*

* Corresponding authors: Marianna Bellardita, e-mail marianna.bellardita@unipa.it

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P6

Experimental Design: study of an industrial reductive amination reaction.

Martina Buccioli[1]*, **Emanuele Farinini**[2], **Riccardo Leardi**[2], **Alberto Moro**[3], **Andrea Basso**[1]

1 – University of Genoa, Department of Chemistry and Industrial Chemistry, Via Dodecaneso 31, 16146 Genoa, Italy
2 – University of Genoa, Department of Pharmaceutical and Food Chemistry and Technology, Via Brigata Salerno (ponte), I-16147 Genoa, Italy
3 – Professional Chemist – Consultant, Passo dell'Osservatorio 1/17, Genoa, Italy

The Design of Experiment is a solid chemometric and multivariate method that allows to study and define the interactions between the variables making a small number of experiments to evaluate many parameters, differently from the "one variable at time" (OVAT) method.[1] Reductive amination reactions play a very important role in pharmaceutical and medicinal chemistry thanks to the presence of many secondary amines among biologically active compounds. About a quarter of C−N bond-forming reactions in the pharmaceutical industry are performed via reductive amination.[2] The methodology reported in this contribution explains the use of DoE to optimize the industrial operating conditions of a reductive amination reaction. This reaction is involved in the first step of a major synthetical route which leads to obtain an important industrial API produced in Bioindustria L.I.M (AL). For this reason, it is significant to achieve high conversion and yield and low impurities. The study started from selecting four different types of reducing agents and three different solvents commonly used in reductive amination, [3] and defining the four-process variable playing an important role in the reaction. A D-optimal design, a full factorial design, and fractional factorial 2^{5-1} and 2^{4-1} designs were used to identify the interaction between the process parameters and the optimal reaction conditions. Furthermore, the experimental variance has been evaluated on optimized conditions.

Keywords: *reductive amination, experimental design, DoE, industrial synthesis*

* Corresponding author: martina.buccioli@edu.unige.it

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P7

Hydrothermal liquefaction of waste PET from densified post-consumer plastic mix

Benedetta Ciuffi[1], Ilaria Agostini[2], Riccardo Gallorini[1], Andrea Maria Rizzo[2], David Chiaramonti[2,3], Luca Rosi[1,2*]

1 - Department of Chemistry "Ugo Schiff", University of Florence, Via della Lastruccia, 3-13, I-50019 Sesto Fiorentino, Italy
2 - Renewable Energy Consortium for R&D (RE-CORD) Viale J. F. Kennedy, 182, 50038 Scarperia e San Piero, Italy
3 - "Galileo Ferraris" Energy Department, Polytechnic of Turin, Corso Duca degli Abruzzi 24, I-10129, Torino, Italy

Hydrothermal liquefaction (HTL) is a promising recycling process for treating plastic waste, enabling the sustainable recovery of high value-added chemicals [1]. This study investigates HTL of PET separated from a densified post-consumer plastic mix mainly used for energy purposes. This is a second raw material composed of 90% polyolefin, while the remaining 10% consists of PET, traces of metals, paper, and glass. A preliminary separation allows to obtain two fractions: one polyolefin and one rich in PET. Two batch experiments were performed in duplicate on the PET fraction in a stainless-steel autoclave at 345°C for 30 and 20 minutes. Both trials resulted in similar yields of the three phases. In particular, the solid yield is around 77% by weight. This phase, after a purification with NaOH 1M, was analyzed by UV-Vis, ^{1}H-NMR and FTIR spectroscopy and consists of terephthalic acid, a product of considerable industrial interest [2]. Furthermore, thanks to the preliminary separation, it was possible to increase the calorific value of the polyolefin fraction from 29.1 to 33.9 MJ/Kg. This fraction can therefore be used to produce fuel. To conclude, the study proved that the hydrothermal liquefaction process is effective for the treatment of densified post-consumer plastic mix.

Keywords: *Hydrothermal liquefaction, plastic waste, PET, terephthalic acid, circular economy*

* Corresponding author: Luca Rosi, luca.rosi@unifi.it

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P8

Lab-scale pyrolysis of wastewater sludge

Massimo Bernardini [1], Reshma Babu [1], Andrea Iebole [1], Gustavo Capannelli [1], Marcello Pagliero [1], Antonio Comite [1]

1- *Dipartimento di Chimica e Chimica Industriale & UdR INSTM di Genova, Università degli Studi di Genova, via Dodecaneso, 31, 16146 Genoa, Italy*

The disposal of wastewater sludge is a significant challenge for our society. Traditional disposal techniques include landfilling, anaerobic treatment, incineration and reuse in agriculture by land-spreading. However, these methods have some environmental issues related to the spread of harmful substances like salts and heavy metals in the soil and the emission of carbon dioxide in the atmosphere.

A promising alternative technology being currently investigated is pyrolysis. This process has several advantages since its products, char, oil and gas, can be useful to fuel generation or as raw materials for production of typical petrochemicals. Pyrolysis is the thermal degradation of matter in the absence of oxygen at temperatures of 350-900 °C. The process temperature determines the product formation: at lower temperature char is the main product, while gas is greater at higher temperature. The decomposition of sludge takes place at different stages of the process due to its heterogeneous nature. The biochar obtained has several applications as solid fuel, in agricultural, or as adsorbent for catalytic purposes. Bioliquid, after removing water, can be utilised as liquid fuel for generation of heat and electricity or for chemical synthesis. Likewise, biogas, especially when obtained at higher temperature, since it contains more hydrogen and methane, can also be used directly as fuel or processed to syngas that can be upgraded to liquid fuel or chemicals production. Since all the pyrolytic products can be utilised, pyrolysis is thought to be a sustainable technique which has great potential for several purposes. In this study, pyrolysis on wastewater sludge that was meant for disposal into landfills was performed. Batch pyrolysis was investigated up to 500 °C and up to 800 °C to study the effect of temperature on the product yields. The main objective was to determine the product distribution and to characterise the char, liquid, and gaseous products. Char was characterised by thermogravimetric analysis (TGA), X-ray fluorescence (XRF) and leaching test, the liquid products by gas chromatography-mass spectrophotometry (GC-MS), Fourier-transform infrared spectroscopy (FTIR) and solubility tests, while the production of hydrogen (H_2), methane (CH_4), ethane (C_2H_6), ethene (C_2H_4), carbon monoxide (CO), and carbon dioxide (CO_2) was monitored during the process using a micro-gaschromatograph.

The results showed that at 500 °C there is higher yield of char and liquid products, while at 800 °C the yields of all products were comparable. However, the gas yield doubled from 500 °C to 800 °C. Among the gases measured, CO_2 was prominent at 500 °C whereas CH_4, and H_2 had higher flow rates at 800 °C. Furthermore, small hydrocarbons such as C_2H_4 and C_2H_6 were observed at 800 °C. From the TGA it was possible to estimate the heating values of the char, showing its potential to be used as a solid fuel. By XRF and leaching test, the presence and availability of phosphates was highlighted. Thus, this char is also suitable as an alternative to synthetic fertilizers. The bioliquid included two phases: a lighter oily phase and a denser aqueous phase. The GC-MS analysis showed that the oily fraction contains larger proportion of phenolic compounds which can have interesting applications as fuels or in the synthesis of organic substances, but treatments for purification and stabilisation will be required.

It can be concluded that the sludge which was to be disposed in landfills could be pyrolyzed and the char can be utilized either as solid fuel or as nutrient supplement in agriculture. The oil fraction of the bioliquid can be further investigated for their ability as feedstock for biofuel production, while gaseous products could be used for power generation or syngas. Thus, pyrolysis looks like a feasible solution for this sludge from an environmental aspect.

Keywords: *pyrolysis, wastewater sludge, biofuel*

* Corresponding author: Antonio Comite, antonio.comite@unige.it

P9

Investigation of MnO_x-WO_3/TiO_2 catalysts for NO-NH_3 SCR

L. Consentino[1*], E. La Greca[1], G. Pantaleo[1], V. La Parola[1] and L.F. Liotta[1]

1 - Institute for the Study of Nanostructured Materials (ISMN)-CNR, via Ugo La Malfa, 153, 90146, Palermo, Italy

Nitrogen oxides (NO_x) produced from mobile and stationary sources are among the major causes of air pollution and are responsible of a series of environmental problems such as acid rain, photochemical smog and the green-house effect [1].
Selective catalytic reduction of NO_x by NH_3 (NO-NH_3 SCR) is the most common method for removal of NO_x emission. Commercial V_2O_5-WO_3/TiO_2 catalysts represent a cheap and robust solution especially with high sulphur content fuels, however, they show good efficiency at high temperatures (300 – 400 °C) forcing the placement of the SCR system close to the engine [2]. In recent years the low temperature (100-200 °C) NH_3-SCR has been widely studied to extend the catalytic performance at low temperature and make the SCR systems more versatile [3]. In addition, the toxicity and easy sublimation of vanadium pentoxide require the design of new vanadium free SCR catalysts, not toxic and able to perform in a wide range of temperature [4]. In this work, a series of Mn-WO_3/TiO_2 catalysts with Mn loading ranging between 1.5 and 12 wt% were synthesized by wetness impregnation of manganese nitrate over WO_3/TiO_2 to evaluate the effect on the conversion of NO_x and selectivity to N_2. Bare MnO_x was also prepared as reference. The best catalyst was compared with a commercial V_2O_5-WO_3/TiO_2 sample. The NO SCR activity was estimated in a fixed bed quartz reactor using a reaction mixture composed of 1000 ppm in NO, 1000 ppm NH_3, 10 %vol in O_2 and He as balance gas at WHSV of 50,000 ml g^{-1} h^{-1}.

Keywords: *vanadium free catalyst, NH_3-SCR, low temperature activity, manganese oxide*

* Corresponding author: Luca Consentino, luca.consentino@ismn.cnr.it

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P10

Preparation of nanopattern catalyst by using nano porous carbon layer with controlled porosity

Palmarita Demoro [1*], Francesco Pio Abramo [1] , Salvatore Abate [1], Gabriele Centi[1], Siglinda Perathoner[1]

1- Department of ChiBioFarAM (Industrial Chemistry), University of Messina, ERIC aisbl and INSTM/CASPE, V.le F. Stagno d'Alcontres 31, Messina 98166, Italy

There is an increasing interest on the synthesis of nanopatterned electrodes for several application in electrocatalysis and more recently plasma-catalysis. In fact, a high concentration of energetic electrons at nanostructured surface could be achieved by using these materials. Electron beam lithography is commonly used for their preparation, in order to access feature sizes between 150 nm and 30 nm. Electron beam lithography provides the highest resolution patterns with a significant amount of flexibility in pattern geometry. Unfortunately, this technique is expensive and non-scalable. The research is oriented towards the use of polymers to allow the formation of a ordered nanomask to be used as a template for the synthesis of nanopatterns. The aim of this work is the preparation of a controlled nano porous carbon layer obtained from furfuryl alcohol-based polymers on titanium foil/mesh and other supports.

The dip coating solution was prepared using furfuryl alcohol, pyrrole, polyethylene glycol and nitric acid. Furfuryl alcohol is a carbon precursor, pyrrole as a binder for the network polymerization reaction and HNO_3 as an acid polymerization catalyst. The amount of pyrrole is the key parameter in order to achieve a controlled nanoporous layer. The polymer-coated titanium mesh was then converted to carbon by heat treatment in an inert atmosphere (Ar).

The shrinkage of the polymer therefore with high temperatures determines an incomplete covering of the titanium mesh. These breaking points would represent the surface on which titanium nanotubes can grow leading to a nanopatterned structure. The effect of both, HNO_3 and pyrrole, on nanoporous carbon layer will be investigated by using Titanium foil and other supports as porous Al2O3 tube, Cordierite Honeycomb and porous stainless steel. Finally, the pores diameter can be further improved by extending the so-called curing time which is the heat treatment in air to form a more cross-linked structure of the carbon precursor [1].

Keywords: nanopattern, titanium, network model

* Corresponding author: Palmarita Demoro, palmarita.demoro@studenti.unime.it

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P11

In-situ activation of Cu-Ni-Fe-Al mixed oxides catalysts for hydrogen transfer in organosolv pulping

I. Z. Awan[1,2,3], O. Gimello[1], T. Cacciaguerra[1], N. Tanchoux[1], S. Albonetti[2], F. Cavani[2], F. Di Renzo[2,*]

1 - ICGM, Université de Montpellier-CNRS-ENSCM, Montpellier, France
2 – Dipartimento di Chimica Industriale Toso Montanari, Alma Mater Studiorum Università di Bologna, Bologna, Italy
3 – Dpt. Chemistry, Lahore Garrison University, Lahore, Pakistan

Organosolv pulping is finding a new revival in second-generation ethanol refineries. Most interest in the conditions of pulping has been addressed to acid hydrolysis and solvation effects. Hydrogen-donor effects in pulping are just starting to receive proper attention. The increase of the H/C and decrease of O/C ratios can open new markets for lignin products. More data about H-transfer on substituted phenolic moieties in realistic conditions are needed to evaluate potential catalysts able to boost oxydehydrogenation in lignocellulose pulping. Copper-bearing mixed oxides from activation of layered double hydroxides (LDH) have been shown to be promising heterogeneous catalysts in organosolv pulping.

In this communication, we present experimental data on the action of non-supercritical methanol on model lignin molecules in the presence of non-noble metals heterogeneous catalysts. Mixed oxides in the Ni-Cu-Fe and Ni-Cu-Al systems, designed for magnetic separation of catalysts, prepared from layered double oxide precursors, were effective catalysts for H-transfer reactions. Relative rates of MPV reaction, O-H and C-C bonds hydrogenation and ether bonds hydrogenolysis have been determined., The oxidation state of copper in the equilibrium catalyst was modified in the reaction medium by the electron-donor activity of the process solvent [1]. Deeper hydrogenation was reached at the increase of the copper content, by successive C-O hydrogenolysis of the aldehyde-alcohol groups and C-C hydrogenolysis of the lateral chains. No hydrogenation of the aromatic rings was observed. The presence of nickel oxide accelerated the hydrogenolysis of a-O-4 bonds. The relative effectiveness of MPV hydrogenation and hydrogenolysis of phenylether bonds can orient the choice of the catalyst in a lignin organosolv environment towards the obtention of products with different molecular weight and level of functionalisation.

Keywords: *biorefinery, lignin, hydrodeoxygenation*

* Corresponding author: F. Di Renzo, francesco.di-renzo@umontpellier.fr

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P12

Polyaniline: reinventing a known polymer

Ermelinda Falletta [1,2*], Daniela Meroni [1,2], Claudia L. Bianchi [1,2]

1 - Department of Chemistry, Università degli Studi di Milano, via Golgi 19, 20133 Milano, Italy
2 - Consorzio INSTM, via Giusti 9, 50121 Florence, Italy

With the rapid expansion of industrial activities, an exponential number of pollutants are being discharged into the environment, leading to a deterioration of the environment and compromising people health. Tons of dyes, heavy metals, drugs, pesticides, VOCs, NOx and many other pollutants every year affect the quality of the entire ecosystem.

The treatment of most of these compounds is challenging because of their resistance to biodegradability and stability towards heat, light, and oxidizing agents. Several technologies have been properly developed (AOPs, filtration, precipitation, etc.) [1]. However, the inherent disadvantages (secondary waste, high operational cost, and complicated procedures) of the methods limit their large-scale application. Among the various remediation techniques, the adsorption-reduction method is a critical way to remediate pollutants contamination because of its high efficiency and cost-effectiveness. Polyaniline (PANI), an interesting innovative conducting polymer, and its composites have been extensively investigated as adsorbents and reducing agents.

Although PANI-based materials have shown very outstanding activity towards both organic and inorganic pollutants removal, some shortcomings have emerged, such as the toxicity of reagents used for the traditional synthesis of the polymer, the fossil origin of the monomer (aniline), etc. Herein, we report innovative methods based on eco-friendly approaches for PANI-based materials fabrication and their application in the field of both water and air remediation [2, 3]. Moreover, the present study proposes new ways of using the polymer for more sustainable solutions.

Keywords: *polyaniline, environmental remediation, eco-friendly synthesis*

* Corresponding author: Ermelinda Falletta, e-mail contact: ermelinda.falletta@unimi.it

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P13

Unconventional photocatalysts for hybrid catalytic processes

R. Fiorenza [1*], A. Nassi [1*], A. Ben Jeannette [1*], V. Spanò [1*], C. Contarino [1], S.A. Balsamo [1], S. Scirè [1]

1 – University of Catania, Department of Chemical Sciences, Viale A.Doria 6, 95125, Catania (Italy).

The recent pandemic situation and the current Russian-Ukraine war highlighted the raw materials exportation crisis. In the EU updated (2020) list of the critical raw materials, new elements were added as the titanium. This points a hard challenge, the research of new, cheaper, and not critical materials that should possess similar performance of the most used ones. To reach this very ambitious goal it is necessary an accurate selection of the catalysts and the modifications of some experimental conditions to favour the increase of the catalytic activity. For this purpose, in the last years our research group focused his attention on the not common photocatalysts, i.e., new or not critical materials instead of the most investigated as TiO_2 or ZnO. Contextually, we have applied different hybrid catalytic approaches to enhance the activity of these materials [1,2]. We have achieved good results (above the 60% of degradation) in the solar photocatalytic removal of emerging contaminants (phthalates) in water combining the photocatalytic features of WO_3 (1% wt) with the high sorption capacity of the $La_2O_2CO_3$ [1]. Similar performances were obtained employing the sonophoto-catalysis and CeO_2-based materials for the removal of the diethyl phthalate, whereas the degradation of phenol was investigated with photocatalytic and photo-Fenton processes using common and cheaper FeO_x-based catalysts. Finally, another important environmental and industrial reaction as the valorisation of the CO_2, was examined with the solar photothermo-catalytic dry reforming (poor studied with this hybrid catalysis) and Ni-based catalysts, whereas the solar photothermo hydrogenation of CO_2 was favoured by the addition of zeolites to the commercial photocatalysts. The high versatility of these multi catalytic approaches and the use of not critical catalysts can be a fascinating route to increase the sustainability and the efficiency of the examined processes.

Keywords: *not common photocatalysts, hybrid catalysis, water purification, CCU*

* Corresponding author: Roberto Fiorenza, roberto.fiorenza@unict.it, Presenters: Armando Nassi, Ahlem Ben Jeannette and Vanessa Spanò.

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P14

Dimethyl adipate: an alternative synthetic route from ketones and organic carbonates

Gabriele Galletti [1*], **Fabrizio Cavani** [1], **Tommaso Tabanelli** [1]

1 – Alma Mater Studiorum – Università di Bologna, Dipartimento di Chimica Industriale "Toso Montanari", Viale del Risorgimento 4, 40136 Bologna, Italy.

In the last decades, the research on industrial processes starting from renewable resources has gathered a constantly growing interest to overcome shortage issues of fossil feedstocks. Adipic acid and its dimethyl ester analogue, dimethyl adipate (DMA), are largely used in many industrial fields, mainly as monomers in the production of Nylon 6,6 and are nowadays produced from benzene through a sequence of polluting reactions. [1] As reported in few examples in literature, a viable alternative for the synthesis of DMA is the reaction between dimethyl carbonate (DMC) and cyclopentanone (CPO) in the presence of both homogeneous and heterogeneous basic catalysts and in discontinuous conditions. This synthetic route is potentially much more sustainable than the traditional one, since DMC can be obtained by direct condensation between carbon dioxide and methanol, whereas CPO can be formed from furfural, a platform molecule derived from hemicellulose, one of the components of lignocellulosic biomasses. [2, 3] In this work, the reaction between DMC and CPO to produce DMA is reported in continuous flow conditions and heterogeneous catalysis, avoiding the use of external solvents by working in DMC excess conditions. The effect of reaction parameters such as contact time and reactants molar ratio has been investigated, and both commercial and synthesized metal oxides (CeO_2, ZrO_2, MgO) have been tested as heterogeneous catalysts. After a stabilization period, both conversions and yields stabilized on values which increased by increasing the contact time in the range tested (1-9 min) and by working with stronger basic catalysts (MgO and CeO_2), reaching values between 15 and 20% for DMA yield, obtained as main product. Moreover, DMC/CPO molar ratio has been tuned in order to find the best compromise between dilution effects and parasite reactions.
Finally, some tests starting from reaction products and intermediates have been performed to confirm the proposed reaction scheme.

Keywords: *dimethyl adipate, dimethyl carbonate, heterogeneous catalysis, continuous flow*

* Corresponding author: Gabriele Galletti, gabriele.galletti5@unibo.it

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P15

Conversion of a rigid polyurethane foam through enzymatic digestion after hydrothermal liquefaction pretreatment

Riccardo Gallorini[1], Benedetta Ciuffi[1], Feliciana Real Fernández[2,3], Cosimo Carozzini[1], Enrico Ravera[1, 4], Anna Maria Papini[1, 3], Luca Rosi[1*]

1 - Department of Chemistry "Ugo Schiff", University of Florence, Via della Lastruccia 3-13, I-50019 Sesto Fiorentino, Italy
2 - CNR – Istituto di Chimica dei Composti Organometallici (CNR-ICCOM), Via Madonna del Piano 10, I-50019 Sesto Fiorentino, Italy
3 - Interdepartmental Research Unit of Peptide and Protein Chemistry and Biology (PeptLab), University of Florence, Via della Lastruccia 13, I-50019 Sesto Fiorentino, Italy
4 - Magnetic Resonance Center (CERM), University of Florence, Via Luigi Sacconi 6, I-50019 Sesto Fiorentino, Italy

Enzymatic digestion is a promising alternative in the upconversion of plastic waste compared to traditional chemical recycling methods, because it warrants the use of milder conditions. However, enzymes are hardly able to penetrate the bulk of the plastic material, thus a pretreatment is necessary to promote the reaction. In this study we investigate hydrothermal liquefaction as a thermal pretreatment of a commercial polyurethane before performing an enzymatic digestion [1]. The feedstock is a rigid polyurethane foam used for model making. The structure and chemical composition of the feedstock were analyzed through FTIR analysis and solid state ^{13}C-NMR. The polyurethane was then subjected to hydrothermal liquefaction using either ultrapure water or KOH as a basic catalyst. Enzymatic digestion was then performed on the organic fraction obtained from both experiments using a lipase extracted from *Candida rugosa* [2]. The LC-MS analysis of the digests shows an increase in signals intensity due to degradation of oligomeric fragments. This new way of recycling allows the recovery of important chemicals such as quinolines and precursor for the polyurethane synthesis, as 4,4'-methylenedianiline.

Keywords: *Hydrothermal liquefaction, Polyurethane, Enzymatic digestion, chemical recycling, circular economy*

* Corresponding author: Luca Rosi, luca.rosi@unifi.it

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P16

Promotional effect of Y on CeO_2, MnO_2 and CeMnOx mixed oxides for NO-SCR by NH_3

Eleonora La Greca[1*], Maria Grabchenko[2], Luca Consentino[1], Daria Savenko[2], Tamara Kharlamova[2], Giuseppe Pantaleo[1], Olga Vodyankina[2], Leonarda Francesca Liotta[1]

1- Institute for the Study of Nanostructured Materials (ISMN), (Italian) National Research Council (CNR), Via Ugo La Malfa 153, 90146 Palermo, Italy
2- Tomsk State University, 36, Lenin Ave., 634050 Tomsk, Russia

Enzymatic digestion is a promising alternative in the upconversion of plastic waste In recent years, large quantities of pollutants are released into the environment from the combustion of fossil fuels; these include nitrogen oxides (NOx) which are a source of serious environmental and human health problems [1]. Selective catalytic reduction (SCR) of NOx by ammonia (NH_3-SCR) is one of the most effective methods used for removal of NOx [2],[3]. The present study focuses on the performance of Yttrium-modified CeO_2, MnO_2 and CeMnOx mixed oxides in the selective catalytic reduction of NOx using ammonia as reducing agent [4]. All the oxides, CeO_2, MnO_2 and CeMnOx (with molar ratio Ce/Mn =1) were prepared by sol-gel method, using citric acid as chelating agent (citrate method). The supports thus obtained were impregnated with yttrium (2wt%), then calcination at 500 °C for 3h. The NO SCR activity was estimated in a fixed bed quartz reactor using a reaction mixture composed of 1000 ppm in NO, 1000 ppm NH_3, 10 %vol in O_2 and He as balance gas at WHSV of 25,000 ml g-1 h^{-1}. The physiochemical properties of the catalysts were obtained by several characterization techniques, such as XRD, H_2–TPR, N_2-physisorption and Raman spectroscopy.

Keywords: *air pollution, SCR, NOx.*

* Corresponding author: Eleonora La Greca, eleonora.lagreca@ismn.cnr.it

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P17

Smart acrylic coatings based on the reversible Diels-Alder reaction

Eleonora Manarin[1,*], Francesca Corsini[1], Gianmarco Griffini[1], Stefano Turri[1]

1- Department of Chemistry, Materials and Chemical Engineering "Giulio Natta", Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Milano, Italy

In this work a thermo-reversible acrylic network was produced *via* a dynamic chemistry approach based on the Diels-Alder (DA) reaction. The strategy to design such DA network was based on the coformulation of a random terpolymer of furfuryl methacrylate (FMA), methacrylic acid (MAA) and 2-ethyl-hexylmethacrylate (EHMA) with a difunctional aliphatic maleimide linker. FMA provides the diene functionality that forms a thermally reversible covalent bond when coupled with the maleimide, MAA favors water dispersion and EHMA works as an internal plasticizer reducing the glass transition temperature of the final material. The FMA content was kept equal to 30 mol% in all the different terpolymers synthesized to optimize the crosslinking density as highlighted in previous studies. Conversely, the relative content of MAA and consequently EHMA functionalities was varied from 60 mol% to 10 mol%. Six different terpolymers were synthesized *via* free radical polymerization. The obtained terpolymers were crosslinked through an aliphatic bismaleimide synthesized starting from 1,6-hexamethylenediamine and maleic anhydride. Among all the candidates, the crosslinked sample denoted as 30:40:30 (*i.e.*, 30 mol% FMA – 40 mol% MAA – 30 mol% EHMA) exhibited excellent thermo-responsiveness, as assessed by DSC analysis. Moreover, an efficient self-repair ability was detected at both the micro and the nanoscale. The study of the self-healing response of this material allowed to highlight three main characteristics of the selected system. First, complete damage repair could only be reached with scratch widths lower than 20 µm. Second, the addition of an external plasticizer (benzyl alcohol) in the final formulation allowed to attain enhanced macromolecular network mobility, consequently increasing the upper limit beyond which only partial scratch healing was observed (from 20 µm to 40 µm). In particular, in these conditions the duration of the healing treatment could also be reduced down to 20 min at 150 °C followed by slow cooling, still preserving a sufficiently effective damage repair. Multiple scratch repair could also be achieved thanks to the proven reversibility of the DA network. Finally, the transparency of the produced coatings was guaranteed, as assessed by UV-Vis spectroscopy, as a result of both the acrylic nature of the terpolymer and the aliphatic character of the BM crosslinker. Based on these evidences, these materials could be considered as promising candidates for the development of smart-resistant water-based surface coatings for outdoor applications.

Keywords: Self-healing, Diels-Alder, water reducible, acrylic polymers

* Corresponding author: Eleonora Manarin, eleonora.manarin@polimi.it

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P18

Oxidation of Alcohols Promoted by Gold in a Microreactor: Kinetic and Modeling Study

Luca Mastroianni [1,2*], Dmitry Murzin[2], Tapio Salmi[2], Martino Di Serio[1], Vincenzo Russo [1,2]

1 – Università degli Studi di Napoli “Federico II, Department of Chemical Sciences, IT-80126 Napoli.
2 - Åbo Akademi, Laboratory of Industrial Chemistry and Reaction Engineering (TKR/PCC), FI-20500 Åbo-Turku, Finland.

The oxidation of primary alcohols to produce aldehydes is a key reaction in organic chemistry [1]. Oxygen represents a clean alternative to the traditionally employed chromium-based oxidants, which are highly toxic for both human beings and environment. Gold nanoparticles are a promising catalyst in selective oxidation processes [2]; hence, a growing interest in catalytic oxidation promoted by gold appeared in both academic and industrial research.
Microreactors have emerged as an exciting technology in process intensification. Their high area-to-volume ratio enables very efficient heat transfer, allowing quasi-isothermal operations in presence of highly exothermic or endothermic reactions. The diffusion of the molecules is rapid because of the micro-metric dimension of microreactor channels, leading to suppression of mass-transfer limitations as the intrinsic kinetics of a reaction is investigated [3].
In this work, the selective oxidation kinetics of methanol, ethanol, propanol and butanol was investigated in a microreactor over Au/Al_2O_3 catalyst. The channels of the microreactor were successfully coated with the catalyst. The properties of both catalyst particles and coating layer were determined with relevant characterization techniques. The influence of reaction temperature, alcohol inlet concentration, oxygen-to-alcohol molar ratio and residence time on both alcohol conversion and product distribution was investigated. To describe the reaction kinetics, plausible kinetic equations were implemented in a pseudo-homogeneous plug flow model, which turned out to be an adequate approximation to describe the flow pattern in the microreactor. An advanced kinetic and diffusion model was implemented to reveal the importance of the intrawashcoat diffusion.

Keywords: *Microreactor, alcohol oxidation, kinetic modelling, gold catalyst.*

* Corresponding author: Luca Mastroianni, luca.mastroianni@abo.fi

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P19

Il Ruolo della Simulazione Molecolare nella Chimica Industriale

Giuseppe Milano

Università degli Studi di Napoli "Federico II, Department of Chemical Sciences, IT-80126 Napoli.

Nella presentazione orale mostrerò alcuni "case of studies" di applicazioni della simulazione molecolare a problemi di tipo industriale. In particolare mostrerò i principali risultati di due linee di ricerca. La prima linea in collaborazione con aziende produttrici di materiali polimerici.[1,2] La seconda motivata dall'interesse dell'industria alimentare per la cristallizzazione dei trigliceridi.[3,4] L'obiettivo generale della relazione è quello di mostrare l'utilità e l'interesse, cresciuto molto negli ultimi anni nel mondo aziendale, di questo tipo di strumento sempre più attuale visto lo sviluppo continuo di hardware potente a basso costo.

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P20

High entropy spinel-structure oxides: synthesis and their electrochemical performance as anodes in Li-ion batteries

Beatrix Petrovičovà[1], Wenlei Xu[2], Maria Grazia Musolino[1,5*], Fabiola Pantò[3], Salvatore Patanè[4], Nicola Pinna[2], Saveria Santangelo[1,5], Claudia Triolo[1,5]

1 – Dipartimento DICEAM, Università Mediterranea di Reggio Calabria, Loc. Feo di Vito, 89122 Reggio Calabria, Italy
2 - Institut für Chemie and IRIS Adlershof, Humboldt-Universität zu Berlin, Brook-Taylor Str. 2, 12489 Berlin, Germany
3 - ITAE - Consiglio Nazionale delle Ricerche (CNR), 98126 Messina, Italy
4 - Dipartimento MIF, Università degli Studi di Messina, 98166 Messina, Italy
5 - National Reference Center for Electrochemical Energy Storage (GISEL), Consorzio INSTM, 50121 Firenze, Italy.

In the latest years, high-entropy oxides (HEOs), a new class of materials, obtained by using configurational entropy-based design approach, have undergone an explosion of interest thank to the possibility of suitably tuning their structural and functional properties. HEOs are single-phase solid solution stabilized in a multi-component system (generally, five or more elements in equimolar or near-equimolar ratio) by a high configurational entropy. The synergistic effects among the constituent species lead to these systems exhibiting an enhanced performance compared to conventional compounds.

This work deals with the synthesis of pure single-phase HEOs with spinel structure under milder conditions (shorter heat treatments at lower temperatures) than the standard solid-state techniques, thus reducing the environmental impact. HEOs are prepared via two routes, sol-gel and electrospinning (by utilizing two different polymers). Ten different equimolar combinations of five metals among Mg, Ti, Cr, Mn, Fe, Co, Ni, Cu and Zn are evaluated. The effect of the synthesis method and conditions on the microstructure, morphology and crystalline phase purity of the produced HEOs is analyzed by using complementary characterization techniques in view of their possible application as electrode materials in rechargeable batteries. The results highlight that the presence of copper or titanium in the equimolar combinations of five metals considered favors the formation of minority secondary phase(s). Electrochemical performance as active anode materials in lithium-ion batteries is preliminarily evaluated on two representative pure single-phase HESOs. To enhance their rate capability and cyclability two possible strategies are proposed and successfully implemented.

Keywords: *high-entropy oxides, spinel oxides, synthesis, electrospinning*

* Corresponding author: Maria Grazia Musolino, e-mail contact: mariagrazia.musolino@unirc.it

P21

Heterogeneous methods for the synthesis of maltose esters

V. Pappalardo, F. Zaccheria, N. Ravasio

CNR SCITEC, c/o Dip. di Chimica via Golgi 19, 20133 Milano

Sugar fatty acid esters (SFAEs) are amphipilic compounds widely employed as active ingredients in several market sectors for the preparation of food, agricultural, cosmetic and pharmaceutical products thanks to theirs excellent surfactants properties. Compared to petrochemical-based ones, SFAEs are neither harmful to the environment nor skin irritants, food-grade, fully biodegradable and non-toxic. Moreover, they are easily digested as a mixture of sugars and fatty acids in the stomach and some of them showed antimicrobial, anticancer and insecticidal activity [1]. These compounds can be produced from renewable agricultural sources (viz sugars, oils and/or fatty acids) by using both chemical and enzymatic esterification. Even if the chemical route is the most widespread at an industrial level, in the last decade the enzymatic route has aroused interest because it is highly regioselective and eco-friendly.

The development of SFAEs from disaccharides, such as sucrose or maltose, allows to the potential formation of complex mixtures of polyesters that are required in several industrial sector. Based on our previous studies about the enzymatic preparation of L-(+)-arabinose-palmitic acid ester [2], we synthesized lauryl-, palmitoyl-, stearoyl-maltose obtaining monoesters as main products in low yields and with long reaction time. In fact, due to the opposite polarities of the substrates the choice of a suitable solvent is the main problem. To overcome these drawbacks, we are studying the activity of mixed oxides following our previous work on the esterification of trimethylolpropane and using solid Lewis acid materials [3]. The results will be compared with those obtained with solid Brønsted acid catalysts, such as the polystyrene sulphonic resins.

Keywords: *sugar fatty acid esters, surfactants, heterogeneous catalysts, renewable sources*

* Corresponding author: valeria.pappalardo@scitec.cnr.it

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P22

Development of novel hybrid materials for heterogenous catalysis

Giuseppe Proietto Salanitri[1,2], Stefano Scurti[1], Sabrina Carola Carroccio[2], Tommaso Mecca[3], Nikolaos Dimitratos[1], Daniele Caretti[1]

1 – Industrial Chemistry "Toso Montanari" Department, University of Bologna, Viale Risorgimento 4, 40126 Bologna, Italy.
2 - CNR-IPCB, Via Paolo Gaifami 18, 95126 Catania, Italy.
3-CNR ICB, Via Paolo Gaifami 18, 95126 Catania, Italy.

Recently, the immobilization of inorganic nanomaterials on polymeric substrates has allowed to develop a wide class of hybrid systems, that combine the benefits of plastic matter such as flexibility, low-cost, mechanical stability, and high durability, with the advantages of their inorganic counterparts [1].
In this optic, the combination of polymer and catalytic active phase could represent a suitable strategy to adopt for a wide range of catalytic applications. [2]
Based on this premise, we have prepared hybrid functionalized macroporous systems with different acid/base properties derived from the decoration of polymeric matrix with metals.
Finally, these hybrid catalysts have been tested for the reduction of 4-nitrophenol to 4-aminophenol to correlate the catalytic activity with the properties of the synthesized system. [3]

Keywords: hybrid materials, heterogenous catalysis, macroporous polymers.

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P23

Magnetic Imprinted Hydrogels for removal and degradation of contaminants from water

Roberta Puglisi [1*], Andrea A. Scamporrino [1], Giuliana Impellizzeri [2], Sabrina C. Carroccio[1]

1 - Institute for Polymers Composites and Biomaterials (National Research Council, IPCB, via P. Gaifami 18, 95126, Catania, Italy)
2 - Institute for Microelectronics and Microsystems (National Research Council, IMM, via S. Sofia 64, 95123, Catania Italy)

Water pollution is a global concern that has attracted many scientists' interest. Anthropogenic activities, including industrials and domestics, cause the introduction of hazardous contaminants (i.e. dyes, pharmaceuticals, chemicals, etc.) in bodies of water, posing a severe threat to human health and environmental quality.[1]

Regarding water pollution, the most promising remediation strategy is the use of adsorbing materials. Among others, hydrogels show remarkable advantages such as high porosity, tunable morphology, cost-effectiveness, and easy handling. In this context, this work provides the design, synthesis, and characterization of new molecularly imprinted polymeric hydrogels containing properly functionalized magnetic nanoparticles, for the selective removal of contaminants from water. The presence of magnetic nanoparticles leads to the safe removal of the hybrid remediation system after the water treatment.[2]

The introduction of organic photosensitizers within the polymer network, warrants the photocatalytic degradation of the pollutants in harmless compounds, under visible light irradiation.[3] To this aim, organic photosensitizers, such as porphyrins or bio-derived porphyrinoids (i.e. chlorophyll), have been synthesized or extracted from natural sources, functionalized, and included within the magnetic imprinted hydrogels. The characterization of the hybrid nano-systems has been performed by means of FT-IR spectroscopy, MALDI-TOF mass spectrometry, thermal analysis and scanning electron microscopy (SEM). Sequestration properties and photodegradation tests towards common dyes and antibiotics were carried out by using UV-Vis spectroscopy, evaluating the degradation rate. Promising results have been obtained using these innovative hybrid materials, paving the way to the realization of highly selective, easily scalable, and sustainable remediation systems.

Keywords: *hydrogels, water, remediation, photocatalysis*

* Corresponding author: Roberta Puglisi, roberta.puglisi@phd.unict.it

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P24

Enhancement of the photocatalytic activity of $BiFeO_3$ nanocrystals by surface modification with metal organic framework.

Luca Pulvirenti[1]*, Cinzia Lombardo[2], Mario Salmeri[2], Maria Teresa Cambria[2] and Guglielmo Guido Condorelli[1]

1 - Dipartimento di Scienze Chimiche, Università degli Studi di Catania and INSTM UdR di Catania, Viale Andrea Doria 6, 95125 Catania, Italy;
2 - Dipartimento di Scienze Biomediche e Biotecnologiche, Sezione di Biochimica, Università degli Studi di Catania, Via S. Sofia 92, 95125 Catania, Italy.

Persistent Organic Pollutants (POPs) (synthetic dyes, pharmaceuticals, pesticides, endocrine disrupting chemicals etc.) are one of the most important groups of pollutants present in urban wastewater. [1,2] POPs cannot be efficiently removed by traditional wastewater treatment with technologies based on biological, physical or chemical approaches. Research efforts have therefore been focusing on the development of new technologies to purify water for consumption. Advanced Oxidation Processes (AOPs) using photocatalytic chemical methods gained much attention over the past decades due to their capability of totally decomposing, in eco-friendly and mild reaction conditions, organic pollutants. [3-5]

In this work, we report on a nanometer hybrid material consisting of nanoparticles of bismuth multiferroic ferrite (BFO) modified through the growth of Metal-organic frameworks of the MIL [6] (Materials Institute Lavoisier) family. The obtained system retains the nanometric dimensions of BFO nanoparticles and the photoactivity tested under natural sunlight irradiation is increased compared to the reference of bare BFO.

Finally, the new BFO@MIL nanocomposite showed also photoactivated antimicrobial properties. When incubated in the dark or after pre-illumination with UV-C, the nanoparticles did not exhibit any bacteriostatic or bactericidal activity whilst under natural sunlight exposure the nanocompound showed a significant decrease in MIC and MBC values compared to bare nanoparticles.

These results suggest that a new material has been successfully developed as efficient photocatalyst and antibacterial agent against a wide range of pollutants and microorganisms to water purification and prevention and control of the persistence of bacterial infections.

Keywords: *bismuth ferrite, MOF, photocatalyst, antimicrobial agent*

* Corresponding author: Luca Pulvirenti, luca.pulvirenti@phd.unict.it;

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P25

Carbon nitride-based catalysts for high pressure CO_2 photoreduction

Gianguido Ramis [1*], Matteo Tommasi [2], Francesco Conte [2], Ilenia Rossetti[2]

1 - Dip. Ing. Chimica, Civile ed Ambientale, Università degli Studi di Genova and INSTM Unit Genova, via all'Opera Pia 15A, 16145 Genoa, Italy
2 - Chemical Plants and Industrial Chemistry Group, Dip. Chimica, Università degli Studi di Milano, CNR-SCITEC and INSTM Unit Milano-Università, via C. Golgi 19, 20133 Milan, Italy

The metal-free polymeric catalyst, graphitic carbon nitride (g-C_3N_4) is a relatively novel catalyst compared to TiO_2. The g-C_3N_4 is characterized by a graphitic 2D type structure and a narrow band gap (on average 2.7 eV) so, in principle it is suitable to be activated by visible light. g-C_3N_4 is commonly prepared via direct thermal condensation of an organic precursor containing carbon and nitrogen, *e.g.* urea, thiourea, melamine, dicyanamide, etc. however the surface area of the produced material resulted low for most of the applications, usually less than 10 m^2g^{-1}. In order to increase the surface area several strategies have been developed, as chemical, mechanical or thermal exfoliation or the use of templates. The aim of this work is to prepare solar sensitive nanophotocatalysts based on g-C_3N_4, as such or loaded over TiO_2 or WO_3, to accomplish the photoreduction of CO_2 at high pressure (up to 20 bar).
Bulk graphitic carbon nitride (g-C_3N_4) was prepared by thermal condensation of melamine. Melamine was placed in a covered ceramic crucible and heated at 2 °C min^{-1} up to 500-600 °C. The resulting yellow powder underwent a successive US treatment, at different US intensity, in order to obtain an exfoliated material showing an increased specific surface area. Binary materials composed of C_3N_4 and TiO_2 P25 or WO_3 were prepared by mechanically mixing both components in different proportions. All the tests for the photoreduction of CO_2 were performed using an innovative pressurized batch photo-reactor, designed to work under pressure up to 20 bar and temperatures up to 90 °C. An increase of pressure showed an increase of the productivity, with a greater effect on the liquid product, *i.e.* formic acid production. Graphitic carbon nitride showed a performance comparable with bare P25. On the other hand, it was observed that when TE was combined with TiO_2 the overall CO_2 conversion to regenerated fuels improved. The composite material showed a much greater productivity of formic acid with respect to both its constituents. The reason must be searched in the interaction between the phases involved, that is titania-carbon nitride-water and synergistic effects among them. The exfoliating ultrasound power directly affected the surface area and structure of carbon nitride, achieving better performance with increasing power. The production of adducts with WO_3 also proved effective to achieve high formic acid productivity.

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Keywords: *Photoreduction of CO_2; Carbon nitride; Photoreactor; Photocatalyst.*

* Corresponding author: gianguidoramis@unige.it

P26

A novel organosolv approach to allow efficient biomass fractionation and successive exploitation

A.M. Raspolli Galletti [1*], D. Licursi [a], N. Di Fidio [1], S. Fulignati [1], R. Baldassari [1], J.C. Parajò[2], S. Rivas[2], C. Antonetti [1]

1- University of Pisa, Department of Chemistry and Industrial Chemistry, Via G. Moruzzi 13, 56124, Pisa, Italy
2- Department of Chemical Engineering, University of Vigo (Campus Ourense), As Lagoas, 32004, Spain

The separation and exploitation of all three main components of lignocellulosic biomass represents a challenging target for biorefinery. In this perspective a novel strategy has been studied for the fractionation and integral exploitation of Arundo Donax *L.* biomass, a feedstock characterized by low cost, large availability, favourable composition and ability to grow in marginal lands unsuitable for agriculture, avoiding any competition with food chain [1]. The adoption of n-butanol (a bioalcohol obtainable form biomass) played a fundamental dual role: as fractionation organosolv agent to separate cellulose, hemicellulose and lignin and also as reagent for the conversion of the obtained cellulose fraction to n-butyl levulinate. The organosolv treatment performed in the presence of diluted acid allowed the one-pot separation of the biomass components in a three-phasic system, obtaining a solid enriched in cellulose, an aqueous phase rich in hemicellulose sugars and an organic lignin-rich phase. A preliminary hot water pre-treatment of the biomass for reducing the content of extractives makes the separation even more effective and allows the further isolation of this component. The organosolv process was preliminarily studied with a One Factor at Time approach and then was optimized with an experimental design in order to determine the joined effect of temperature, time and catalyst concentration on organosolv fractionation. Under the optimized conditions a valuable solid with about 80 wt % of cellulose was obtained and at the same time two liquid fractions, aqueous and organic, for further exploitation of soluble hemicelluloses and lignin derivatives respectively. In particular, the occurred solubilisation of lignin allows its conversion adopting hydrogenation or oxidation processes or it can be recovered as solid by reprecipitation. The recovered cellulose-rich solid was exploited with n-butanol itself in the one-pot alcoholysis reaction to n-butyl levulinate, an emerging blending molecule for diesel fuel and a valuable chemical intermediate [2]. A preliminary optimization of the main reaction conditions (temperature, reaction time, acid catalyst concentration) was performed: in the presence of diluted sulphuric acid, butyl levulinate yields of 40 mol % were reached, a promising result in comparison with the literature data.

Keywords: *organosolv, biomass, butyl levulinate*

* Corresponding author: Anna Maria Raspolli Galletti, anna.maria.raspolli.galletti@unipi.it

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P27

PescaPlastica experience: a virtuous model of management and use of marine litter collected in the Mediterranean Sea to produce fuel

Paolo M. Riccobene[1*], Angela Cuttitta[2], Emilio Giacalone[3], Sandro Dattilo[1], Luciano Falqui[4], Andrea A. Scamporrino[1], Sabrina C. Carroccio[1]

1 – CNR IPCB Institute for Polymers, Composites and Biomaterials – Via P. Gaifami, 18 Catania, CT
2 – CNR ISMED Institute for studies on the Mediterranean - Via F. Parlatore, 65 – Palermo, PA
3 – O.P. di Trapani e Isole Egadi - Via Cristoforo Colombo 8 – Trapani, TP
4 - Greenertech Srl - Via Nicola Fabrizi, 21, Catania, CT

In the last decade, the problem of marine litter has increased worldwide [1]. Tons of plastic debris are dispersed daily in the sea, causing several problems that directly and indirectly affect human beings. In this context, our work aims to identify a virtuous model of management and use of marine litter, focusing attention on the valorization of plastics *fished* at sea. For this purpose, in collaboration with local fishing communities, plastics present in Trapani sea area were collected, separated, and analyzed by thermogravimetry analysis (TGA), Pyrolysis-gas chromatography/mass spectrometry (Py-GC/MS), and Matrix-Assisted Laser Desorption/Ionization – Time of Flight (MALDI-TOF) to obtain thermal profiles and typologies of each polymer constituting the mix.
The standardized feed received from the collection areas was pyrolyzed at different temperatures, achieving the suitable parameters to produce the best bio-oil yield [2]. The obtained results will be used in the pyrolysis plant demonstrator allowing the processing of mixed plastic waste with low sorting and pre-treatment intervention, converting them into energy.

Figure 1. Project logo and Concept.

Keywords: Plastic Litter, Pyrolysis, Blue Economy, Sustainability.
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* Corresponding author: Paolo M. Riccobene, paolomaria.riccobene

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Electrocatalytic reduction of CO_2 on single crystal Cu_xO-based gas-diffusion electrodes

A. M. Ronsisvalle [1*], D. Giusi [1], C. Ampelli [1*], G. Centi [1], S. Perathoner [1]

1 – Department of Chemical, Biological, Pharmaceutical and Environmental Sciences (ChiBioFarAm), University of Messina, ERIC aisbl and CASPE/INSTM, V.le F. Stagno d'Alcontres, 31 - 98166 Messina (Italy)

The conversion of CO_2 into value-added chemicals and fuels by using renewable energy sources is one of the most promising routes to relieve the energy crisis and environmental issues caused by excessive exploitation of fossil fuels. In this regard, artificial leaf-type devices are an attractive solution to convert CO_2 and H_2O using solar light (or renewable electrical energy). However, to be sustainable and cost competitive, the use of critical raw materials or noble metals should be avoided for the construction of electrodes [1]. The main challenges related to CO_2 electroreduction are the high overpotentials needed to perform the multi-electron transfers and the poor Faradaic Efficiency (FE) and product selectivity. Atomic-level understanding of the active sites and transformation mechanisms under realistic working conditions is a prerequisite for the rational design of electrocatalysts with high selectivity. Among the earth-abundant materials, copper oxide (Cu_xO) is a suitable candidate for CO_2 electroreduction. In this work, we synthesised single crystal Cu_xO nanoplatelets by a facile hydrothermal approach at low temperature starting from copper (II) chloride dihydrate $CuCl_2$. For comparison, we used different precursors by adding NaOH or LiOH. The as-prepared electrocatalytic materials were deposited by spray-coating onto carbon-based gas-diffusion electrodes and then assembled in a homemade compact electrochemical device for CO_2 reduction tests. The electrodes were fully characterized by XRD and SEM, and by Electrochemical Impedance Spectroscopy (EIS) to evaluate the influence of diffusion phenomena on the electrocatalytic performance. Results showed the high activity of these electrodes in CO_2 reduction in near-neutral pH conditions, due to the predominantly exposed {001} reactive facets and the thin nanoplatelet architecture. Moreover, we observed a different selectivity depending on the precursor used during the preparation, i.e. Na or Li. The catalyst prepared with LiOH was more selective to carbon monoxide (CO), evidencing a FE to CO of 45% (with a current density of 9 mA cm^{-2} at –0.4 V vs. RHE), while using NaOH as the precursor led to a higher FE to formate.

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Keywords: *CO_2 conversion, copper oxide, single crystal catalysts, Li precursor*

*Corresponding authors: A.M. Ronsisvalle, angela.ronsisvalle@iusspavia.it; C. Ampelli, ampellic@unime.it

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Kinetic investigation of ethyl levulinate ketalization with glycerol

Vincenzo Russo [1*], Francesco Taddeo [1], Roberto Esposito [1], Riccardo Tesser [1], Martino Di Serio [1]

1 - Department of Chemical Sciences, University of Naples Federico II, Via Cinthia, 80126-Naples, Italy

Levulinic acid esters (LAEs) are a class of compounds easily obtained from renewable raw materials such as cellulose, hemicellulose or starch. The ketalization reaction of levulinate alkyl allows to obtain products with very interesting applications for the chemical industry such as in the field of solvents, lubricants, plasticizers as levulinic ketals can be easily functionalized and are thermally and chemically stable [1]. Recently, we proved that ion exchange resins and zeolites can promote the reaction, H-Y zeolite the most active. The aim of the work is the investigation of ethyl levulinate ketals synthesis reaction kinetics promoted by H-Y zeolite. A kinetic investigation was conducted with this catalyst to retrieve the parameters needed for a possible scale-up procedure to produce LAEs ketals in a continuous device. Different experiments were conducted varying the main operation parameters to retrieve the kinetic information. Fluid-solid mass transfer limitation can be considered negligible working at stirring rate greater than 600rpm. Experiments were conducted varying the catalyst loading, obtaining a proportionality coefficient with the catalyst bulk density of 0.5, indicating strong influence of intraparticle mass transfer limitation. Experiments conducted at different temperatures allowed to obtain an apparent activation energy value of 30kJ/mol, value in-line with the occurrence of intraparticle mass transfer limitations. From these data, a reaction heat of 21kJ/mol was obtained. Some experiments were conducted in a milli-reactor demonstrating the feasibility of the operation in flow. Experiments were conducted at different temperatures and residence times and interpreted using the kinetic parameters retrieved in batch, showing the validity of the approach.

Keywords: *ketalization, ethyl levulinate, glycerol, kinetics, modeling*

* Corresponding author: Vincenzo Russo, v.russo@unina.it

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Hydrogels from biomass waste valorisation: design and applications

Antonella Salvini [1,2,4*], Donatella Giomi [1,2], Camilla Parmeggiani [1,3], Sara Baracani [1], Samuele Visi[1], Silvia Giorgi [1], Rodorico Giorgi [1, 4**]**

1 - University of Florence, Department of Chemistry "Ugo Schiff", via della Lastruccia 3-13, 50019 Sesto Fiorentino (FI), Italia)
2 - Laboratorio congiunto VALORE", via della Lastruccia 3-13, 50019 Sesto Fiorentino (FI), Italia)
3 – European Laboratory for Non Linear Spectroscopy, via N. Carrara 1, Sesto F.no
4 - CSGI, via della Lastruccia 3, 50019 Sesto Fiorentino (FI), Italia

The exploitation of renewable materials coming from biomass is a strategic goal for the chemical industry to reduce the depletion of fossil resources resolving, at the same time, waste disposal issues. On the other hand, the availability in the market of advanced biocompatible hydrogels could be really significant for their use in environmental applications as adsorbents in water remediation, biomedical field or conservation of cultural heritage.

Based on this, new hydrogels were obtained from the valorization of waste biomass recovered from food processing and agro-industries or from the lignocellulosic waste. In particular, cellulose and other polysaccharides were recovered from biomass waste using specific protocols that have been optimized based on the different biomass composition. Mechanical, physical and chemical treatments were optimized based on the kind of biomass studied. Pullulan, an oligosaccharide material deriving from the enzymatic transformation of starch [1], was also used as starting material. Then the crosslinking reactions were achieved employing multifunctional reagents as crosslinkers. In particular, several commercial formulations containing hexamethylene diisocyanate trimers were studied and showed a different solubility or dispersion ability and their performances as cross-linking agents were compared.

The gels were characterized by the calculation of the gel fraction (G%), in order to calculate the yield of the gelation process. The EWC (equilibrium water content) parameter allowed to know how much the gel is hydrophilic, through the calculation of the water contained in the system.

The images acquired with SEM (Scanning Electron Microscope) allowed to obtain information on morphology and structure of the gels and in particular to study the presence or absence of porosity inside.

Preliminary application tests were carried out to evaluate the performance in the cleaning of works of art and other possible commercial applications.

Keywords: *biomass valorization, polysaccharides, hydrogels, crosslinkers*

* Corresponding author: Antonella Salvini antonella.salvini@unifi.it
** no kinship is present between the co-authors

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P31

Palladium supported over carbon nanotubes catalytic system for Green diesel production

Stefano Savino [1*], Michele Casiello [1], Antonio Monopoli[1], Caterina Fusco [2], Lucia D'Accolti [1], Angelo Nacci [1]

1 – University of Bari "Aldo Moro", Chemistry Department, via Orabona 4, 70125 Bari, Italy
2 – CNR—Istituto di Chimica dei Composti Organometallici (ICCOM), Bari Section, via Orabona 4, 70126 Bari, Italy

Nowadays biomass can be considered a cheaper, more sustainable and abundantly available energy resource to replace fossil fuels. For this reason, the synthesis of green diesel is analyzed in this project, involving the use of a new generation palladium-based catalyst supported on previously functionalized Multi-Walled Carbon Nanotubes (MWCNT) [1].

In particular, the MWCNTs used have cavities with dimensions between 50 nm and 90 nm, a size sufficient to allow their functionalization and therefore the deposition of Pd also on the internal walls of the support. The internal functionalization allows generating a zone with a high local concentration of catalyst, thus leading to greater efficiency compared to conventional catalysts [2].

The investigated process is the hydrodeoxygenation (HDO) reaction of triglycerides for the synthesis of 2nd generation biodiesel (biodiesel with a totally hydrocarbon composition). Furthermore, it was tried the use of two additives such as glycerol and formic acid capable of providing in situ hydrogen required for the reaction. Given that formic acid and glycerol are considered industrial waste products, their use as hydrogen generators greatly increases the value of this process in a perspective of circular economy.

The results of this project, although entirely preliminary, highlight the effectiveness of carbon-based catalytic systems in these processes.

Keywords: Biodiesel, Carbon Nanotubes, Catalysis

* Corresponding author: stefano.savino@uniba.it

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P32

Adsorption of ibuprofen on activated carbon: experimental data validation using adsorption dynamic intraparticle model (ADIM)

R. Tesser, M.E. Fortunato, M. Hmoudah, R. Paparo, M. Trifuoggi, V. Russo, M. Di Serio

1 – University of Naples Federico II, via Vicinale Cupa Cintia, 26. IT-80126 Napoli

The increase of Emerging Contaminants - ECs (which include pharmaceutically active compounds, personal care products, artificial sweeteners and endocrine disrupting chemicals) in wastewaters and the concern about the unknown long-term effects of their accumulation in the environment brought researchers to a growing awareness about the need to improve existing technologies and to develop new strategies for their removal from wastewater [1]. Ibuprofen [2-(4-Isobutylphenyl) propionic acid] is a nonsteroidal anti-inflammatory drug (NSAID) that is primarily used as a painkiller and antipyretic and it is one of the most prevalent ECs found in the environment, with detected levels in wastewater treatment plants influents which go from the tens to the hundreds µg/L [2]. Over the years, adsorption was proved to be efficient methods for wastewater treatment due to their high efficiency and low costs, also thanks to the employment of solid materials which can be easily separated and reused: for this reason, this technology is promising for the removal of ECs from waters. In this work, the kinetics of adsorption of commercial activated carbon towards ibuprofen was investigated and described using adsorption dynamic intraparticle model (ADIM) [3]. Although the adsorption capacity of activated carbon was widely studied in the literature, the corresponding kinetics models are limited. By fitting the kinetic data obtained from a series of adsorption tests conducted in a thermostated, stirred glass-jacketed reactor, it was possible to obtain important parameters like the surface diffusivity, DS, and the fluid-solid mass-transfer coefficient, km. In particular, the mass balances have been developed by considering for both the external and internal mass transfer diffusion limitations, solving the dynamic partial differential equations (PDEs) system along the radius of the sorbent particles, considering both the fluid andsolid phases that constitute the sorbent particle. The equilibrium isotherm model was predicted using Fruendlich model.With the validated model, the influence of some operating parameters on the adsorption behavior was studied, namely, solution bulk density, solution initial concentration, stirring rate and temperature effect.

Keywords: Biodiesel, Carbon Nanotubes, Catalysis

* Corresponding author: stefano.savino@uniba.it

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Heterogeneous catalyzed ketalization of ethyl levulinate with glycerol

Rosa Turco [1,2*], Francesco Taddeo[1], Riccardo Tesser[1], Martino Di Serio[1], Vincenzo Russo [1]

1 - Department of Chemical Sciences, University of Naples Federico II, Complesso Universitario di Monte Sant'Angelo,-Naples, Italy
2 - Institute for Polymers, Composites and Biomaterials, National Council of Research, Pozzuoli, Italy

Alkyl Levulinates (Als) are important platform molecules, easily derivable from biomass, which can be converted into valuable chemicals [1]. The reaction of Als with alcohol leads to the formation of the ketals, which have found widespread application as flavorings, plasticizing agents, and fuel additives. Mineral acids are usually applied as catalysts for the reaction. The use of heterogeneous catalysts could overcome environmental and technological issues, reducing downstream costs [2]. This work is aimed at the synthesis of ethyl levulinate ketals, through an acid heterogeneous catalysis. For this purpose, different acid solids have been investigated as active and selective catalysts, including ionic exchange resins and zeolites. Beta zeolite showed the highest activity and selectivity towards the desired products.

Keywords: *Ketalization, Ethyl Levulinate, heterogenous catalysts*

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Synthesis of new defoamer agents and characterization in cement formulations

R. Vitiello[1]*, M. Ruocco[1], F. Taddeo[1], R. Turco[1], R. Tesser[1], M. Di Serio[1]

1 – University of Naples Federico II, Chemical Science Department Complesso Universitario di Monte Sant'Angelo,-Naples, Italy

The production of cementitious formulations involves the addition of chemical additives essential for the optimization of many properties. The additives of greatest interest are superplasticizers, these are polymeric dispersants added during the preparation of concrete itself in order to improve the rheology and workability of the formulation [1]. The use of superplasticizers has many advantages but, nevertheless, during mixing with concrete there may be an undesirable increase in air content, thus allowing the development of foam, deriving from the surfactant properties of the superplasticizer. This can adversely affect both mechanical properties and machining, therefore, the use of an antifoaming agent is necessary [2]. Due to the insolubility of the antifoaming agent in the medium there could be a phase separation with respect to the aqueous solution of superplasticizer, making it ineffective and compromising the storage of the superplasticizer-antifoam formulation [3]. Therefore, it was decided to use a system sensitive to the change in pH. The experimental approach initially focused on the synthesis of esters through an acid-catalyzed esterification reaction between esters, derived from biomass (betaine, alkyl levulinate) and fatty alcohols of different chain length and of different nature. The reaction products were analysed by a ^{1}H-NMR analysis. Subsequently, the stability of antifoaming agents in a superplasticizer solution was studied through foaming tests in accordance with the Ross-Miles method, while their efficiency in cement systems was evaluated through Flow Table tests. In this work, it has been identified that a chain length comprised between 12 and 14 carbon atoms resulted to be the optimal range.

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Keywords: defoamer agent, esterification reaction, biomass.

* Corresponding author: rosa.vitiello@unina.it

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