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Camerino
28 September 2018

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Camerino, 28 September 2018

Dear Colleagues,

I am happy and proud to present the 6^{th} edition of the Scientific Day of the School of Science and Technology (SST) of the University of Camerino. This booklet contains an unavoidably incomplete collection of the wide and diverse research activity carried out within the School I have the honor to lead.

Our SST is a unique environment in which the five Divisions - Chemistry, Computer Science, Geology, Mathematics, and Physics - organize and stimulate cross-disciplinary and multidisciplinary research activities.

Postdoc, PhD students, and young researchers are the protagonists in the Scientific Day and I firmly believe they will be the driving force in continuing our tradition of a lively scientific debate and cross-fertilization among different areas and research fields. The activities presented during the Scientific Day will also provide a wide spectrum of research approaches, ranging from societal application - frequently carried out in close collaboration with companies and local institutions- to fundamental science challenges, often organized in collaboration with the most prestigious international institutions.

The 6^{th} Scientific Day edition is the first after the October 2016 earthquake. For this reason, it will also be the first edition not to take place in the stunning Ducal Palace four-sided portico. Our School, together with the whole University, has promptly responded to this terrible event: this Scientific Day represents one of the many examples of how we will continue to strengthen the University of Camerino's centennial tradition as a leading center for Science and Culture.

The Dean of the SST
David Vitali

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Chemistry

Design, synthesis, reactivity, biological and catalytic applications of functionalized bis(pyrazolyl)acetate copper complexes

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Bis(azol-1-yl)carboxylic acids are convenient starting materials for the synthesis of neutral heteroscorpionate systems based on bis(azol-1-yl)methane linked by acetate, acetamide or thioacetamide moieties. Recently, we have focused the research work on the development of two bis(pyrazol-1-yl)acetates, [HC(COOH)(pz)$_2$] (LH) and [HC(COOH)(pz^{Me2})$_2$] (L^{2}H) and the related analogues esterified with several alcohols such as methanol, ethanol, isopropanol and hexanol. All ligands have been used to obtain the copper(II) complexes starting from Cu(II) acceptors and to synthesize the related Cu(I) complexes by reaction of $Cu(CH_3CN)_4PF_6$ and 1,3,5-triaza-7- phosphaadamantane (PTA), tris(hydroxymethyl) phosphine (thp) and triphenylphosphine (PPh_3) with LH and L^{2}H ligands in acetonitrile solution. In addition, based on the observation that copper nitroimidazole conjugates have recently shown additive or synergistic selectivity for tumor hypoxia compared to their individual components,[1] Cu(I) and Cu(II) complexes of 5-nitroimidazole conjugated heteroscorpionate ligands have been prepared. The new ligands L^{MN} and L^{2MN} have been synthesized by direct coupling of preformed side chain acids LH and L^{2}H with 5-nitroimidazole and their coordination chemistry has been investigated towards Cu(I/II) acceptors.[2] Finally, LH and L^{2}H have been bioconjugated with the NMDA receptor antagonist (±)-(6,6-diphenyl-1,4-dioxan-2- yl)methanamine and the resulting ligands have been used to synthesize the related copper derivatives, potentially acting through synergistic mechanisms of action due to the presence of the NMDA ligand and copper in the same chemical entity.3 Several new copper complexes as well as the corresponding uncoordinated ligands were evaluated for their cytotoxic activity against 2D monolayer cultures of multiple human cancer cell lines and the most promising derivatives also against 3D-cultured HCT-15 colon cancer spheroids. The investigation of their catalytic activity in the radical allylic oxidation of olefins, using the Kharasch-Sosnovsky reaction, is also in progress.

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Investigation on the method to quantify tocopherols in vegetable food matrices

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Vitamin E is a term used for a family of compounds that are mainly represented by tocopherols ($\alpha, beta, \gamma$ and δ), and tocotrienols, compounds naturally present in plants and in their products. They belong to the group of fat-soluble vitamins and α-tocopherol is the most biologically active form of vitamin E.[1]

Due to their hydrophobic characteristics, vitamin E compounds are closely associated with lipids in food and they have the essential role of protecting unsaturated lipids from oxidation, preserving them in biological systems and in foods.[2]

The objective of this research work was to determine the content of tocopherols ($\alpha, beta, \gamma$ and δ) in several vegetable food matrices (i.e. coffee powder and vegetable oils) and especially to assess and compare different sample preparation methods by analyzing the lipid extract as such or its isolated unsaponifiable matter through normal-phase high performance liquid chromatography (NP-HPLC). It was also assessed the possible role of the atmosphere composition during the saponification reaction by carrying out the reaction under inert atmosphere (nitrogen) or not. Pyrogallol and 2,2,5,7,8-pentamethyl-6-chromanol were used respectively as anti-oxidant and internal standard.

A fluorescence detector coupled to NP-HPLC was used to identify and quantify these molecules, after their separation, taking advantage of specific emission wavelengths of tocopherols. Preliminary results will be presented and discussed.

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Improved method to quantify squalene in extra virgin olive oil

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Squalene is a triterpene having several interesting properties, e.g., it is an antioxidant, it has anticancer activities and it increases immune response in vaccine administration.[1–3]

The present work was aimed to develop and validate a rapid and efficient method to quantify squalene in olive oil (one of the richest food sources of squalene), by gas chromatography coupled with flame ionization detector (GC-FID) and to apply the method to determine squalene content in extra virgin olive oils (EVOOs) from Marche Region (Italy) and to EVOOs from large scale distribution retail.

The developed method makes use of a transmethylation of the oil sample in order to allow the GC analysis of squalene together with fatty acid methyl esters, thus avoiding the separation of squalene from saponifiable fraction. The optimized conditions allow to perform the analysis with high sensitivity, short time and with instruments and materials usually available in most of the laboratories. The proposed method was validated by determining linearity, repeatability, reproducibility, recovery at three fortification levels, limit of detection and limit of quantification.

Results from the method validation and from the application of the method to niche EVOOs and to EVOOs from large scale distribution retail will be presented.

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Development of a rapid and reliable method for short chain fatty acids extraction and analysis

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Short chain fatty acids (SCFAs) are the main products together with carbon dioxide, methane, hydrogen and heat, that derive from the bacterial fermentation of polysaccharides, oligosaccharides, proteins, peptides and glycoproteins precursors in the colon.[1] Their determination is useful in many fields of research, since they have currently attracted much consideration because of their beneficial physiological effects. For example SCFAs can positively change the composition of the intestinal flora[2] and they have been associated with reduced risk of some diseases like irritable bowel syndrome, cardiovascular disease and cancer.[1]

The aim of this study was to develop a rapid and reliable method to extract and quantify these analytes (acetic acid, propionic acid, butyric and isobutyric acid) from different biological samples, i.e. rat feces and fermentation fluids.

Briefly, the homogenized samples are acidified with sulphuric acid, added with an internal standard and extracted several times with ethyl ether. The obtained ether solution is analyzed by direct injection in splitless mode using gas-chromatography coupled to flame ionization detector (GC-FID). The method is simple, versatile and sensitive and compared to other procedures e.g. involving solid phase micro-extraction[3], it is quicker and more precise.

The method was validated assessing linearity, interday and intraday repeatibility, recovery, limit of detection and limit of quantification with satisfactory results.

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The use of "geopolymers" for the treatment of tannery wastewaters

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The treatment of tannery wastewaters has been the subject of many studies throughout the years due to the complexity of the waste: a mixture of several pollutants, both anionic and cationic as well as organic macromolecules which are very hard to dispose all together[1]. Geopolymers are a class of inorganic binders obtained by alkali activation of aluminosilicate powders at room temperature[2]. The geopolymerization process leads to a cement like matrix that transforms the hazardous waste into inert material, including Cr^{3+}, $SO_4{}^{2-}$, Cl^- and H_2S. In this work we make use of two different matrixes, one metakaolin3 and one unfired clay, to asses their possible use in an industrial environment.

Leaching tests were performed after 28 days and after 3 months of consolidation showing no leaching and confirming the successful inertization.

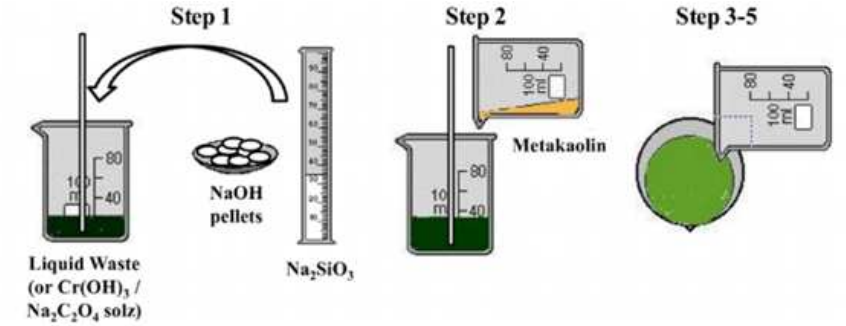

Fig. 1. Geopolymer preparation steps.

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Synthesis and Characterization of a Si/V2O5 Nanocomposite as Anode Material for Lithium-Ion Batteries

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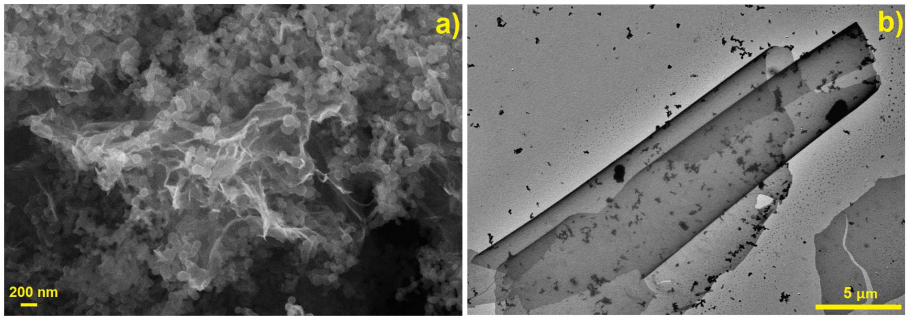
The synthesis and the complete structural and electrochemical characterization of a Si/V_2O_5 nanosheets[1] nanocomposite, as anode material for Li-ion batteries, are here reported. This approach, aimed at mitigating morphological instability issues commonly plaguing Si-based anodes, consists in wrapping silicon nanoparticles in V_2O_5 nanosheets prepared by a simple and direct reaction between H2O2 and crystalline V_2O_5 (c-V_2O_5)[2]. The electrode processing involves the use of the alternative binder Polyacrylic Acid (PAA) and ethanol as solvent[3]. In addition to the non-toxicity of the used solvent, this binder system provides better mechanical stability to the electrode. The electrolyte formulation has been evaluated, by using Vinylene Carbonate (VC) as reduction-type additive, in order to maximize cycling stability and performances. Preliminary results report specific capacities of 932 mAh g^{-1} and 759 mAh g^{-1} after 50 cycles at 500 mA g^{-1} and 1000 mA g^{-1}, respectively.



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Vanillin-Templated Fe2O3 as Alternative Anode Material for Lithium-Ion Batteries

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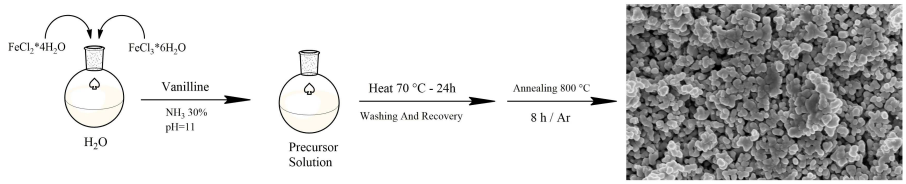
Transition metal oxide (TMOs) are alternative candidate anode materials characterized by low-cost, environmental benignity, and high theoretical specific capacities[1]. Despite this, TMOs are plagued by critical volume expansion during charge/discharge cycles, which compromise electrode perfomances and safety[2]. Developing tailored material morphologies together with an optimized electrode processing could help to minimize this phenomenon. In this work, Fe_2O_3nanoparticles have been synthesized using vanillin as soft templating agent and morphologically, structurally and electrochemically characterized. Furthermore, a Polyacrylic Acid/Ethanol binder system was used instead of the traditional Polyvinylidene Fluoride/N-Methyl-2-pyrrolidone binder system, which is toxic and expensive. This material showed excellent rate capabilities and a remarkable gravimetric capacity of 700 mAh g^{-1}after 250 cycles at 500 mA g^{-1} specific current.



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β-Nitroacrylates: useful starting material for the synthesis of heterocycles

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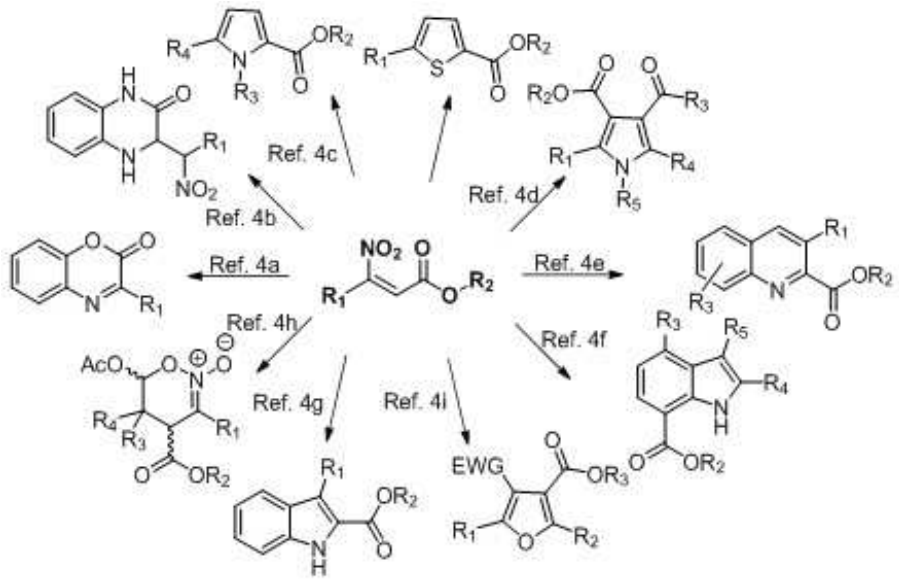
β-Nitroacrylates constitute a class of electron-poor alkenes bonding two electron-withdrawing group in α- and β-positions. The presence of these two functionalities makes their chemical behavior more fascinating with respect to the conventional conjugated nitroolefins and β-nitroacrylates valuable precursors of a plethora of highly functionalized materials.[1,2] In this context, our research group has recently investigated their application as precious building blocks of key heterocyclic derivatives such as pyrroles, thiophenes, indoles, quinolines, furans (Figure 1), cores of a wide number of biological active molecules present in the 59% of small-molecules drugs (U.S. FDA).[3] Significant synthetic results will be described in the poster.



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Facile route for the synthesis of activated hard carbon as anode material for lithium/sodium ion battery

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Hard-carbon (non-graphitized carbon) is considered as one of the most promising anode materials for both lithium-ion batteries (LIBs) and Sodium-ion batteries (SIBs) due to its low cost and high theoretical capacity.[1] A unique feature of this material is its simple synthesis from low cost natural materials, also including food waste such as apple peels and olive leaves. However, the development of novel synthetic routes to meet the required properties is still a challenge.[2] In the present study, various samples of hard Carbon were synthesized through chemical acid activation of various natural materials.[3] The nanostructures are studied by X-ray diffraction (XRD), Raman spectroscopy and scanning electron microscopy (SEM) methods. The lithium/sodium intercalation capabilities of various carbon materials have been compared based on their electrochemical performance.

The highest initial capacity of apple peel derived product as LIB and NIB (at 1C) were 395 and 350 $mAhg^{-1}$, respectively. For NIB, olive leaves derived materials deliver a retained capacity of 100 $mAhg^{-1}$ after 350 cycles at 1 C, and for LIB, materials show high specific capacity of 500 mAhg-1 at 1C. The good electrochemical performance indicates that this low-cost hard carbon could be a promising material for dual functional batteries. Additionally, the sodium-ion storage behavior of HC is deeply analyzed using galvanostatic intermittent titration and cyclic voltammetry technologies.

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NMC Cathode materials synthesis for lithium-ion batteries

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Nanotechnology is an emerging approach to develop efficient and enhanced batteries including the most popular lithium-ion ones. The importance of cathode materials in LIBs are tremendous since the LIBs are still cathode limited in design and useful capacity. $LiNi_{0.33}Co_{0.33}Mn_{0.33}O_2$ have been used for years in lithium ion batteries for stable and high energy density cathodes.[1,2]

In this study, we have developed a facile approach for the synthesis of cathode materials with enhanced properties to improve electrochemical performances of LIBs. Prospective cathode materials NMC for a lithium-ion batteries were successfully synthesized through a novel synthetic method including a citric acid-assisted sol-gel processing followed by drying and calcination at different temperatures.[3,4] The surface morphology was characterized by scanning electron microscopy (SEM). The phase and structure of the nanostructures were revealed by X-ray diffraction spectroscopy (XRD). The electrochemical properties were also studied. As determined by galvanostatic potential limitation (GCPL) the $LiNi_{0.33}Co_{0.33}Mn_{0.33}O_2$ materials gave an efficient charge/discharge behavior at 1C and C/5, in the voltage range between 3V and 4.6V. Moreover, the cyclic voltammetry and charge/discharge curves showed good electrochemical stability with a capacity retention of 75% after 180 cycles. These promising preliminary results obtained with this synthesis open possibilities for performance improvements by structure doping or surface enhancement.

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Synthesis, Characterization, Structural and Optoelectronic Properties of Trimetallic Monovalent Coinage Metal Acceptors

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Supramolecular adducts can be formed by the stacking of acidic or basic cyclic trimetallic coinage metal(I) complexes and the corresponding Lewis bases or acids.[1,2] In this work, reactions between the π-acidic cyclic trimetallic coinage metal(I) complexes $[Cu(\mu\text{-}3,5\text{-}(CF_3)_2pz)]_3$, $[Ag(\mu\text{-}3,5\text{-}(CF_3)_2pz)]_3$, $[Au(\mu\text{-}3,5\text{-}(CF_3)_2pz)]_3$ and $[Ag(\mu\text{-}3,5\text{-}(NO_2)_2pz)]_3$ with TTF, DBTTF and BEDT-TTF give rise to twelve 1 : 1 and 1: 2 new binary donor-acceptor adducts stable in bench conditions (where pz = pyrazolate, TTF = tetrathiafulvalene, DBTTF = dibenzotetrathiafulvalene, and BEDT-TTF = bis(ethylenedithio)tetrathiafulvalene). These novel binary donor-acceptor adducts and their properties have been characterized by solid-state structural and spectroscopic analyses. This series of binary donor-acceptor adducts have been found to exhibit remarkable supramolecular structures in both the solid state and solution, whereby they exhibit supramolecular stacked chains and oligomers, respectively. The supramolecular solid and solution binary donor-acceptor adducts also exhibit superior shelf stability under ambient lab storage conditions, and remarkable magneto-optoelectronic properties, as highlighted by 1H and 19F NMR, UV-Vis-NIR spectroscopy, FTIR, and computational investigations. The potential applications of this new class of supramolecular binary donor-acceptor adducts in molecular electronics, including solar cells, (super)conductors, magnetic switching devices, and field effect transistors (FETs) are overviewed.

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Sustainable Strategies for the Synthesis of Polyfunctionalized Heterocycles with Potential Biological Activity from Acyclic Precursors

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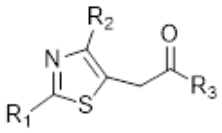
Considered the real cornerstones of medicinal chemistry, thanks to their versatility and physicochemical properties, heterocycles or heterocyclic cores are present in most pharmaceutical products currently on the market. Among the wide range of biological activities, heterocyclic compounds have a considerable active role as anti-bacterial, anti-viral, anti-fungal, anti-inflammatory, and anti-tumor drugs.[1] Despite the extensive literature focused on the synthesis and functionalization of heterocycles, there remains a great need for further advances in this area,[2] and the development of sustainable strategies for obtaining scaffolds of functionalized heterocycles is still a challenge for organic chemists.

In this scenario, we developed the cyclization of acyclic precursors that contain linearly encoded functional groups for giving targets with high regio- and stereochemical control.[3] By finely tuning the reaction conditions, we were able to synthesize important build blocks in medicinal chemistry such as acylaminothiazoles (1) under catalyst-free conditions, in good to excellent yields without any purification step for the whole process.[4] Similarly, we developed the synthesis of polysubstituted isoxazoles (2) under solvent-free conditions with solid supported $CeCl_3 \cdot 7\ H2O/NaI$ catalytic system.



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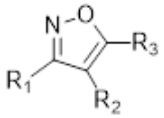

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Characterization of the distribution of TiO2, resin and pigment within a water-based paints.

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The TiO_2 is a very versatile material and used in numerous fields like from cosmetics to paints.

Titanium dioxide for its high refractive index it is used mainly as pigment white in paints, plastics and cement from construction and as matting for colored paints; for this reason, it is also commonly called "Titanium white".

The TiO_2 is used in paints for its photo catalytic activity[1] and self-cleaning inside the acrylic paints.[2] Within the coating all components are located in solution through a delicate balance of forces and through factors such as temperature, pH, humidity and type of dispersants used can be altered.[3]

In the system, where the balance is unchanged, we have that all components are dispersed evenly; the resin surrounds titanium, pigment and any other raw materials present. When balance fails the tinting strength varies so the resulting color will be different. In this particular case was performed a complete study on the morphology by SEM-XRD where was also made a primary mapping for observing the dispersal of elements; AFM, to observe whether the surface is homogeneous; Electron Microscope through which it was observed the phenomenon of lack of pigment dispersion.

The analyses have revealed that the troubled paint samples present an inhomogeneous particle distribution where the resin is located in greater quantities on the bottom and titanium floats on the surface. For the other ones it may be noted that pigment dispersion in general was not good because you have areas of accumulation. While in the sample without problems the dispersion of all components was perfect.

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Efficient Lewis Acid Systems for the A3 Coupling reaction

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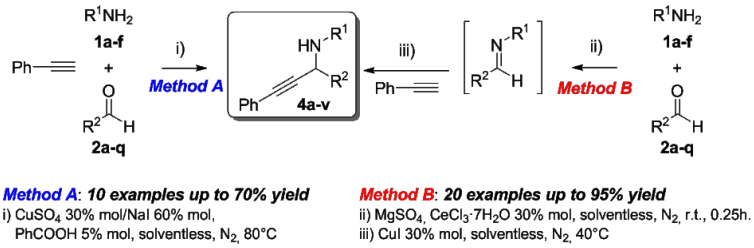
Propargylamines are an attractive class of molecules because of their particular molecular skeleton, that contains an amine group located in β-position to an alkyne moiety suitable for many chemical transformations. In recent years they received a growing interest as key intermediates for several biologically active compound, natural products and also different heterocycles.[1,2] Our goal was the development of green and simple methodologies for the synthesis of secondary propargylamines by Lewis acid catalyzed or promoted A^3 reaction among aldehydes, alkynes and primary amines, that are in general less applied in such reactions because of their lower reactivity. In particular, we studied two different pathway: the $CuSO_4$/NaI system (Method A) in one pot fashion and the $CeCl_3$/CuI system (Method B) in one pot/two steps way (Scheme 1).



Heptahydrated $CeCl_3$ is reported to be an excellent catalyst for many useful organic transformation as the synthesis of imines. Its efficacy as Lewis acid is enhanced in the presence of inorganic iodides and being cooper the transition metal of choice for A_3 reactions, CuI was used.[3]

Also the $CuSO_4$/NaI couple has revealed to be an interesting Lewis acid system as an alternative to $CeCl_3$/CuI system which allow the formation of CuI *in situ* by quantitative spontaneous reaction that takes place in few seconds.[4]

Typically, $CuSO_4$/NaI catalysed reactions are faster than $CeCl_3$·7H2O/CuI reactions, but suffer of some disadvantages, such as lower yields, and a narrower applicability. When a chiral starting aldehyde was used, an opposite diastereoselectivity was observed with the two different promoters. The amine in general has no effect on the reaction outcome.

The relevant Glaser coupling drawback observed in the CuSO4/NaI system conditions has been suppressed by adding some benzoic acid, and has not been observed with the $CeCl_3$/CuI system.

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Contamination of polymeric materials with natural molecules

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Discoloration of white or light-colored polymer materials has long been a serious problem affecting polymers in the industry. Discoloration is usually associated with a degradation process.[1] During degradation, different chemical reactions occur along the polymer chains.[2]Polyesters are of great importance as fiber materials and several studies have been conducted on the dyeing with natural colorants such as tannins through a transesterification reaction. Tannins play an important role in the textile applications by improving the affinity of fibres towards different dyes. By mixing with other natural dyes it gives different shades like yellow, brown, grey and black.[3] The dyeing of polyesters must be achieved only in the textile industries, but must be avoided in other application such as food contact materials. The discoloration of polyesters is observed when it is put in contact with substances that contains tannins in specific conditions. Wine and tea in basic conditions are the main responsible for this problem. The synergistic action of three factors: the tannins, the basic conditions and the metals presents in wine and tea, is the main cause of discoloration in polyesters. The transesterification reaction is catalyzed by various metals: aluminium, tin, magnesium, calcium, zinc, titanium and by the basics condition that increase the chemical reactivity of tannins. When one of these factors are not in combination with the others the discoloration of polymers is not achieved.4

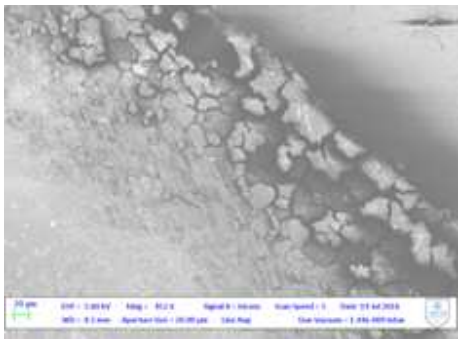

Figure 1 - SEM image.

The SEM images shows that the discoloration of polyesters lead to a surface modification of the polymer (fig. 1).

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Two different graphene: which of the two is the best in the photocatalytic activity of TiO2 under visible light?

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Since the discovery by Fujishima and Honda of the photochemical water splitting, TiO2 photocatalysis has been widely studied for its environmental applications [1]. However, despite the potential of TiO_2 as photocatalyst, there are two limitations in its application. The first is that TiO_2 is not photoactive under visible light because of its wide band gap (3.2 eV); the second is the fast recombination rate of electron-hole pairs that decrease the efficiency of photocatalytic reactions [2]. A possible solution for these limitations is the doping with various species such as graphene. Graphene is an ideal nanomaterial for doping TiO_2 thanks to its large specific surface area, high transparency and the formation of Ti-O-C bonds that extend the visible light absorption of TiO_2. Furthermore, electrons are easily transported from TiO2 to graphene sheets and the electron-hole recombination is considerably reduced, enhancing the photocatalytic efficiency [3].

In this study, graphene (GR) [3] and reduced graphene oxide (rGO) dispersion, that were prepared and characterized in our laboratory by two different eco-friendly methods, both were used with TiO_2 nanoparticles for the preparation of nanocomposites supported on polypropylene [4] (PP@GR-TiO_2 and PP@rGO-TiO_2). These nanocomposites were tested as visible light photocatalysts for the visible light photodegradation of Alizarin Red S (ARS) in water as target pollutant. The use of the two different graphene combined with TiO2 demonstrated that their presence led to significant improvements for ARS adsorption on the catalyst surface and related photodegradation under visible light irradiation when compared to only TiO_2. All the results was compared and discussed.

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$CeCl_3.7H_2O$ in the Non Biomimetic Synthesis of Biologically Active Compounds

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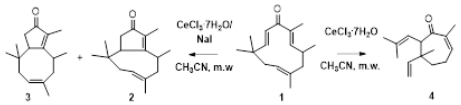
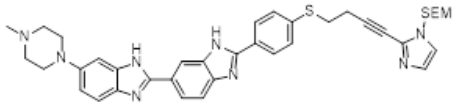
Cerium is the most abundant element in the series of the lanthanides, and one of the more widely used in organic chemistry, both for academic and industrial applications.[1] The low toxicity, ease of handling and low cost, have made $CeCl_3$ an extremely interesting compound for organic chemistry applications.[2] In the recent years, $CeCl_3.7H_2O$, as efficient Lewis acid promoter, has found a plethora of applicability in several organic reactions and in the formation of new carbon-carbon and carbon heteroatom bonds in important biological active compounds.[3] Against this background, we developed two non Biomimetic synthetic protocols, based on $CeCl_3.7H_2O$ promoting system, to reach the formation of two biologically active cyclic compounds.

The first regards a Nazarov type annulation starting from the monocyclic humulane trienone zerumbone (1) obtaining polycyclic sesquiterpenoid skeletons (2-4) which are not reported as natural products and have a significant active role as anti-bacterial, anti-inflammatory, anti-oxidant and anti-tumor drugs.[4]



The second concerns a chemo- and regioselective oxidative cyclization to reach the bis benzimidazolic scaffold characteristic of a innovative Hoechst molecule type which are useful for many different therapeutic and diagnostic purposes due to the capability to bind DNA and microRNAs.[5]



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A Flipped Classroom - IBSE Aapproach for the Teaching of Chemical Concepts

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In the AY 2016/17, a research/action on the learning of chemical concepts, using the Flipped Classroom [1] pedagogical model and the IBSE approach (Inquiry Based Science Education) emphasizing the 5E Learning Cycle [2], has been undertaken by two school teachers in collaboration with UNICAM PLS project (Scientific Degrees National Plan). The Flipped Classroom repurposes class time by reversing traditional teaching (lecture-style teacher centered sessions and home self-study) so content is delivered outside the classroom where the student can adjust the learning process to his own acquisition style. Thus, in-class time can be devoted to in-depth revision, under teacher's guidance. After an initial online teacher training on chemical concepts and methodologies using UNICAM Moodle platform, the students' activities were planned according to the five-phase sequence of Engage, Explore, Explain, Elaborate, Evaluate. During phase III, the class conducted a lab activity adopting a semi-structured IBSE [3], where some steps of the laboratory procedures were devised by the students. Finally, the impact on skills upgrade was evaluated. The result analysis shows an overall benefit, both in terms of skills acquired by pupils and acquisition of the new teaching practice by teachers.

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Development and validation of analytical method to monitor the BVOC emission in Sibillini National Park using TD-GC-MS.

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Biogenic volatile organic compounds (BVOCs), are a heterogeneous group of molecules with a wide range of functions useful for plants and, consequently, for the whole ecosystem and the environment[1]. A rapidly and inexpensive analytical method is presented that is based on the use of thermal gas-chromatography (TD-GC-MS) to monitor BVOCs released by Juniperus Communis in Sibillini National Park. Hexanal, Toluene, α-Pinene, 4-Terpineol and β-Caryophyllene have been used as standard compounds. This method showed a good sensibility (limit of detection ranges between 10-19 pptv for all compounds except for Hexanal that is 100 pptv), repeatability (RDS% within 11%), precision (recovery higher than 85%) and selectivity. We collected samples in situ from April 2016 to September 2017 almost once for months. The compounds have been identified using Kovats retention indices (RI) and quantified with the response factor (RF) for different class of compounds. All samples have been correlated with temperature and humidity values. The results show higher emission in April (flowering period) and at particular condition of temperature (24Â°C). These results are comparable to the data found in the literature about emissions of Juniperus Communis, confirming the validity of the developed method[2][3].

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Compatibilization of Rubber/EVA Compounds for Sole Applications

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Due to market competitiveness, outsole industry has to improve itself. This challenge, combined with the risk of a failure in the market, strongly promotes the research of innovative polymeric materials or blends. TPU (ThermoPlasticUrethane)/PU (PolyUrethane) and rubber/PU are the most known example of polymeric blends used in soles for technical applications.[1] In last years, EVA (Ethyl Vinyl Acetate) has gathered great attention due to its great resistance to UV light and ozone and to its density: the acetoxy content has a strong influence because on one hand the acetoxy functional group reduces the polyethylene crystallinity degree, on the other, the polymer assumes a more amorphous and rubber-like character as the acetoxy content increases.[2,3] "Rubber" indicates a wide range of materials used in outsole factories for fashion and/or technical articles. Natural and synthetic rubbers are important due to their versatile characteristics: SBR, IR and BR have good physical and process properties, compatibility and they are generally economic; NBR, EPDM, CR (Chloroprene rubber) are used in particular outsole products that have special requirements.[4] However, rubber and EVA don't have a high compatibility degree each other; in fact, the aim of this study is to find an appropriate formulation that ensembles the advantages of rubber (good physical-mechanical properties) and EVA having 18% acetate content (optimal chemical resistance). Density, abrasion and tear resistance, breaking strength and elongation are evaluated according to the ISO regulations. IR spectra and SEM images have also been recorded.

In more than fifty years of activity, Delta Spa is deeply involved in research of innovative materials for outsole products. Delta Spa has become one of the most important reality in this field: starting from PU and rubber to EVA and TR soles, the outstanding quality made it an international leader in outsole market.

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Graphene doped nickel oxide for solar conversion

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Dye Sensitized Solar Cells (DSSCs) represent a low-cost alternative device respect to the conventional Silicon photovoltaics systems[1]. DSSC based on p-type semiconductor convert sunlight to electricity by the absorption of a dye on p-type semiconductor nanomaterial, in this case NiO, that act as photocathode, with a Pt-counter electrode and a redox electrolyte at interface. In NiO-p-DSSC a hole injection occurs into the NiO-valence band from the excited dye adsorbed on the nanostructured material[2]. The scientific research focused its attention on NiO p-type-DSSC due to its potential use in tandem DSSC, in which the p-type NiO photocathode is combined with the n-type TiO_2 photoanode; unfortunately, the performance of tandem device is lower respect the n-type device connected to the lower efficiency of the p-type photocathode[3]. One strategy to improve the performance of NiO-p-DSSC is modifying and optimizing the semiconductor in order to improve the photovoltage of the device, metal doping can increase electrical conductivity and tune the band gap energies of the semiconductor by increasing charge carrier transport, charge density and Fermi level[4].

In this study, graphene was synthetized in our laboratory by glucose thermal reduction and, to improve the charge transport and the efficiency of NiO-p-DSSC, NiO layers were doped with different amount of graphene to decrease the back reaction responsible for the recombination process and increase open circuit photovoltage of the device. Graphene was characterized by UV-vis and XPS, p-NiO DSSCs were analyzed by Current-Voltage measurements and Incident Photon-to-Current conversion Efficiencies (IPCE) and the NiO layers, with and without graphene, have been characterized by FE-SEM and Raman analysis.

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Computer Science

Sensor positioning with Geometric Constraint Solving Using Relative Distances

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In this research, we want to find a positioning process for sensors in a wide area starting from incomplete and noisy distance measure. During the sensor positioning process, various problems may arise, such as errors in the calibration of the sensors themselves, but also problems relating to the difficulty of covering a large area as best as possible or still positioning a large number of sensors in an optimized manner.

The problem of determining node positions is generically known as *network localization*[1]: the absolute node positions (with respect to a local or global reference frame) need be estimated from partial relative measurements between nodes, that is, each node may measure the relative position (angle and distance, or distance only) from a set of neighbor nodes, and the global absolute positions of all nodes need be estimated from this information[2].

Starting from node distances we investigate an approach to formulate mathematical and geometrical relations between nodes to place them in a given area. The purpose is to find a solution to the network localization problem with imprecise and incomplete distance information that satisfy distance constraints and that can be further used to optimization.

In range localization it is usually assumed that some nodes, called anchor nodes or beacons, know their position with respect to an absolute reference frame, while the remaining nodes have to be localized in this given frame. Anchor-free approaches also exist. In them the lack of an absolute reference frame imposes the localization to be relative and a node of the network is usually assumed to be at the origin of the reference frame.

We are working to an anchor-free method of localization. The approaches used in this research are based several optimization techniques[3,4,5] as genetic algorithms and on some numerical optimization methods to minimize errors in the positioning such as the Least Squares method or the Lagrangian Multiplier method. Using these techniques, it is possible to position a large number of sensors in a specific area, even having incomplete or wrong distances between the sensors themselves.

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Exploiting IoT sensor data using Machine Learning techniques for developing a Predictive Maintenance system

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The purpose of this research is to employ IoT sensor data[1], the use of which is rapidly increasing in industrial plants, to create a combination of machine learning models which can be used as the basis of a Predictive Maintenance System[2].

In Industry, when a machine failure occurs the entire production system need to be stopped for hours or days to perform a corrective maintenance of the fault. Predictive Maintenance System aims to report when a failure is about to happen in order to take all the necessary precautions to prevent it from occurring3. In addition to preventing faults, this system need to be capable of detecting when irregular behavior, like energy waste happen. Since these irregular behaviors are difficult to be recognized by humans, Anomaly Detection algorithms need to be used4. In addition to this, we must also fix some threshold values that indicates the normal behavior of a system.

The methodology used in this research for the implementation of this kind of system is Data Driven, so called because it has as its object the study of historical data to understand what are the recurring factors that cause a failure. Using Machine Learning techniques, it is possible to create models that can predict what will be the value of a IoT Sensor data in the near future, using historical, time series data of the sensor taken into consideration. Since the data come from different sensor, a preprocessing phase is the first essential step to build a predictive model, then the model need to be trained and tested in order to find the Machine Learning algorithm with the best accuracy. When a model for a specific dataset is created, it is possible to make prediction. The result of this prediction can be used, in the first place to make a comparison between the predicted values and real values of the sensors, so as to verify in real time if there is an anomaly, otherwise, if the prediction returns an anomaly itself, the system can report that an irregular behavior is about to happen.

The domain investigated is related to HVAC and energy consumption in buildings where multiple solutions based on artificial intelligence and statistical approaches can be used to model the behavior of the system and to recognize anomalies[5].

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BProVe: a User Friendly Business Process Verifier

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The successfulness of a company does not reside only on the quality of final products and services that it provides. It also resides on the optimization of all the activities that lead to the realization of those products and services. Ensuring a proper execution of activities, highlighting bottlenecks, suggesting ways to improve the overall process, are tasks that reside in the area of Business Process Management. One way to optimize a Business Processes is to gather all the information that concern the involved activities and represent them in the form of a Process Model by means of a standard and graphical notation (e.g. BPMN and EPC).

One of the most spread notation for carrying out this task is BPMN. Despite the widespread of this notation, techniques to verify correctness properties such as: absence of deadlocks, reachability of certain states, correct activities execution order, are still not directly supported. Usually, a translation from BPMN to other formalisms is required together with the use of third-party tools for performing such property verifications. This negatively affects users which face the risk of losing themselves into technicalities without finding what they are really looking for: an easy to use tool that does all this job automatically. BProVe is a tool based on years of studies[1] which, by the definition of an Operational Semantics for the BPMN notation, brought the possibility to apply formal methods techniques directly over models. BProVe comes as an open-source Web-Service which has been already integrated into modeling environments like Eclipse[2] and APROMORE[3]. BProVe proved its effectiveness passing several tests over thousands of models providing correct responses to the verification of a well-known property in the area, the so-called soundness property. An empirical study on the usability of BProVe is envisioned as upcoming work.

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Use of Three-Valued Spatio-Temporal Logic for the Analysis of Smart Systems

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Smart systems are large-scale, physically-distributed services where different kinds of data-collection sensors are used to supply information employed to efficiently manage assets and resources, and provide efficient operations. These systems are increasingly pervasive and interact extensively with their environment. System components are arranged in logical/physical space and their position. It is thus crucial that unexpected and possibly dangerous situations be avoided. Hence, there is a strong need of techniques to guarantee that systems are trustworthy.

Stochastic analysis has proved to be effective and useful for many systems which encompass behaviour that is not entirely predictable. Moreover, probabilistic model checking has been successfully used to support system analysis. However, this approach is often limited by the state-explosion problem. To overcome this problem, simulation-based approaches have been used to provide summary information about the satisfaction of properties providing estimated values that include intrinsic uncertainty.

In [1,2] a novel Three-Valued Spatio-Temporal Logic (TSTL) has been proposed to take into account uncertainty and to enrich the summary information. TSTL integrates temporal and topological operators, borrowed from [3], that allow us to verify spatio-temporal properties using a three-valued approach. For instance, TSTL has been used to evaluate the efficacy of a control measure for fire spread. The fire spread in a specific area will happen with probability under a given threshold over time. This analysis permits identifying the locations that are at highest risk, because they are surrounded by locations with high probability of burning.

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Process-based Modelling towards the Simulation of Long-distance Electrodynamic Interactions of Biomolecules

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Our work is focussed on the computational study of the molecular interactions in biological systems. We hypothesise the use of process algebras to highlight the relation between the complexity of the functions carried out by a biological entity and the type of interactions tying the elementary units that compose its structure. This approach is intended to define predictive models able to generate new knowledge, on the system itself, complementary to the one obtained via empirical methods.

We investigated the way in which the interactions between nucleotides determine the three-dimensional conformation of RNAs and hence their functions. With the aid of formal models based on CCS process algebra, we compared the folding process of proteins with the one performed by RNAs. We formally proved the existence of an abstraction level in which these two kinds of processes show a congruence in their behaviour[1]. Such result allows us to identify and model the distinguishing features of the studied biological processes only on the basis of the known properties of the interactions that bind the nucleotides (in RNAs) and the amino acids (in proteins).

We are also working on an application of the proposed modelling approach to the studies carried out at the CPT (Centre de Physique Théorique, Aix-Marseille University) on the long-distance electrodynamic interactions of biomolecules[2]. The main idea is to develop a simulator able to solve the problem of the possible interpenetrations of the represented molecules. It would be also intended to yield information on the temporal evolution of the molecular interactions.

Applications of our approach in modelling the processes involved in gene expression would allow the identification of mutations in human gene pathologies; on the other hand, simulations of protein interactions would be the basis of in-silico studies of the formation of protein aggregates in neurodegenerative diseases.

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Collaboration vs Choreography Conformance in BPMN 2.0: from Theory to Practice

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The BPMN 2.0 standard [1] is nowadays largely used to model distributed informative systems in both academic and industrial contexts. The notation makes possible to represent these systems from different perspectives. A local perspective, using collaboration diagrams, to describe the internal behaviour of each component of the systems, and a global perspective, using choreography diagrams, where the interactions between system components are highlighted without exposing their internal structure. In this paper, we propose a formal approach for checking conformance of collaborations, representing possible system implementations, with respect to choreographies, representing global constraints concerning components'interactions. In particular, we provide a direct formal operational semantics [2, 5, 7] for both BPMN collaboration and choreography diagrams, and we formalise the conformance concept [3, 6, 8-9] by means of two relations defined on top of the semantics. To support the approach into practice we have developed the C4 tool [4]. Its main characteristic is to make the exploited formal methods transparent to systems designers, thus fostering a wider adoption of them in the development of distributed informative systems. We illustrate the benefits of our approach by means of a simple, yet realistic, example concerning a traveling scenario.

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DaRe

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The Data Science Project to Re-image education (Da.Re.) is part of the Erasmus+ program funded by the European Union. The final goal of this project is to design an innovative study curriculum in Data Science. Each member of the consortium carried out a survey in their own country to know the state of the art of data science according to three main directives: university training paths of all levels, skills sought by companies (Market needs) and new desired skills for facing future challenges (Training needs). The results of the survey show the need, by small and medium-sized enterprises (SMEs), of people skilled in data analysis but also aware of the specific domain in which the companies operate. This is a class of professional not well served by existing educational or training offerings.

The Da.Re. curriculum is intended to shape such a figure who has been called a 'bridge person'. A bridge between the specific domain of the companies and the capability to analyze data is necessary.

The Da.Re. curriculum design has two parts: 80 hours online education followed by 70 hours face-to-face education with experts from companies. The idea is that the online education provides students with the technical knowledge and skills needed to do the handson training at the two-week 70-hours face-to-face residential school. By combining online and face-to-face education, Da.Re. can combine the best of MOOCs and the boot camp approach to provide new, useful and sustainable data science education in Europe.

The pilot course, that was launched in August 2018, represent the basis for defining the final contents of the curriculum.

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Neural Networks for Next Day Prediction Energy Consumption: the Leaf Lab Case Study

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Energy management have always been a great challenge in our society. The prediction of energy consumption of offices, apartments and even entire buildings could be the key for helping in reducing the energy utilization, in designing and sizing renewable energy and storage systems [1,2]. In this work we compared a combination of different architectures parameters and paradigms in order to forecast the next day energy consumption.

Our data are the recordings of the energy consumption and external temperatures in a period of two years, of the Leaf Lab, a building belonging to the Loccioni Group that kindly provided us those data. Feedforward, with different topologies, and Recurrent neural networks with a long short term memory unit have been used [3,4].

We trained and tested our networks using the data of the first year and then we forecasted the daily consumption of the next one. We evaluated each network in terms of the Mean Absolute Percentage Error (MAPE), the Mean Squared Error, (MSE) and the Root Mean Squared Error (RMSE). We got that the recurrent neural network performed better that the others obtaining a MAPE of 22%, a MSE of 18.03 and a RMSE of 4.25.

In this work, contrary to what is reported in the literature, validation has been carried out over a long period (one year); moreover, the data provided were noisy and had a large number of "holes". Despite this, our network managed to contain the error in almost all the predictions; only some of these presented a very high error.

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Early Detection of Depressive Mood: The TREE Project Lab Case Study

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Depression is recognized as one the major cause of illness especially for patients in the rehabilitation phase from spinal traumas [1]. The early automatic detection of depressive states, using environmental sensors placed in rehabilitation facilities, is important both for the clinicians who can intervene in a targeted manner and for the patient who, in this way, does not risk aggravating the pathology. Unfortunately in the literature very few works are reported in this field; moreover, most of the studies are done on older people at home: an elderly person is considered healthy as long as he can carry out daily activities as usual, without significant deviations from the normal daily routine. In order to monitoring deviations techniques such as SVM, fuzzy logic, Bayesian methods, decision trees, ANN and HMM are used [2,3].

The aim of this work is defining and then implementing an algorithm to monitor the domestic behavior of patients of all ages, in the rehabilitation phase, which could hide clues to the development of depressive pathologies. In particular, what we want to monitor daily activity, focusing on the actions performed by patients, on the number of hours of rest, on mobility within the facilities, on the predisposition to go out and socialize, on the use of environments and appliances. Data collected from ad-hoc surveys is going to be used, too. The resultant algorithm will be a support in clinical diagnosis.

This work is part of the Tailored Rehabilitation for the Engagement and Empowerment of chronically disabled people Project (TREE), funded by The Marche Region (POR MARCHE FESR 2014-2020 "SALUTE E BENESSERE"). The aim is to create a model of social and health service in the areas of rehabilitation, monitoring and assistance, which can respond to changes in care needs.

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Alignment tree for RNA pseudoknots

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Ribonucleic acid (RNA) is a linear polymer of nucleotides arranged in a sequence referred to as a backbone. This sequence is made of four different types of nucleotides, known as Adenine (A), Guanine (G), Cytosine (C) and Uracil (U), and folds back on itself creating complex shapes, known as secondary structures. RNA secondary structures comparison is a fundamental task in several studies, among which RNA structure prediction and evolution. The comparison can currently be done efficient only for pseudoknot-free structures due to their inherent tree representation.

In this work, we introduce an algebraic language to represent both pseudoknot-free and pseudoknotted motifs that induces RNA trees permitting an efficient comparison of RNA secondary structures of any kind. For each structure, a unique extended RNA tree is derived from a tree grammar based on operators concatenation, nesting and crossing. From an extended RNA tree, an abstraction is defined in which the primary structure is neglected. The resulting structural RNA tree allows us to defined a measure of similarity calculated exploiting classical tree alignment algorithms.

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A Loop Grammar to Understand the roles of miRNAs in the Tumor Cell

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A miRNA is a small non-coding RNA molecule that regulates gene expression. Current studies showed that miRNAs may function both as oncogenes and as tumor suppressors, but not revealed the precise conditions that cause miRNAs to alter gene expression of the cancer cells. In this study, we introduce a context-free grammar, *Loop Grammar*, that formalizes the primary and secondary structure as a composition of loops, corresponding to concatenation or nesting of hairpins. We also formalize the *concatenation* and *nesting* on *fatgraphs*, oriented surfaces with boundary, and we define a *Surface Loop Grammar*, whose algebraic expressions uniquely identify such surfaces associated to given RNA structures. The Loop Grammar has been used to model tumor and healthy miRNAs of the mir-515 family, and we observed that the mutations of elements of primary structure involved in loops formation changed the secondary structure of tumor miRNAs. The Surface Loop Grammar is useful to classify RNA structures in terms of loops and relations among them.

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MIDA: Multiple Instances and Data Animator

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The increasing adoption of modelling methods contributes to a better understanding of the flow of processes, from the internal behaviour of a single organisation to a wider perspective where several organisations exchange messages. In this regard, BPMN collaboration [1] is a suitable modelling abstraction. Even if this is a widely accepted notation, only a limited effort has been expended in formalising its semantics, especially for what it concerns the interplay among control features, data handling and exchange of messages in scenarios requiring multiple instances of the interacting participants. In our study [2], we face the problem of providing a formal semantics for BPMN collaborations including multiple instances, while taking into account the data perspective. Beyond defining a novel formalisation, we also provide a BPMN collaboration animator tool called MIDA [3] that permits to understand the precise behaviour of BPMN models [4,5]. MIDA shows the model execution by means of flow of tokens, following the rules induced by our BPMN formal semantics. MIDA turns out to be an effective supporting tool for enhancing the understanding of BPMN collaborations and debugging errors that can easily arise in modelling them.

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Combining Machine Learning with Knowledge Engineering to Detect Fake News in Social Networks

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Fake news is a type of yellow journalism or propaganda that consists of deliberate misinformation or hoaxes spread via traditional print and broadcast news media or online social media. Fake news is as old as the news industry itself-misinformation, propaganda, hoaxes and satire have long been in existence. Detection of fake news gained worldwide popularity after US presidential elections 2016 and now a day it has become a hot issue. The importance of fake news can easily be understood as per the report published by PEW Research Centre. 38% adults often gets news online, 28% rely on website/apps & 18% rely on social media. Overall 64% of adults feel that fake news causes a great deal of confusions [1]. As per our research question "*How would one accurately distinguish between fake and non fake articles on social networks by combining machine learning with knowledge engineering?*"

To answer this question our idea is to combine learning from data and engineered knowledge in order to combat fake news detection in social media. A new text classification algorithm approach shall be developed which will classify the text as soon as news is published online into the classes' fake, non-fake, unclear. These days the most actively researched classifier is Support Vector Machine (SVM) that can classify the text [2]. After text classification the next step for identification of fake news is stance detection, which categorizes the news into four categories: agree, disagree, discuss and not related. For this purpose we will apply different algorithms to check the stance of the other social sites. In next step we will apply fact checking that will refine the results. While classification can be based on cross validation using deep learning methods based on text and metadata like source, author, topic and claim wise [3], fact checking uses engineered knowledge in order to analyse the content of the text and compare it to known facts. At the end the three sub results will be combined in order to differentiate the fake and non fake news in social networks.

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Geology

Chemical Characterization of Construction and Demolition Waste

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Construction and demolition (C&D) wastes account for highly heterogeneous materials, as concrete, rocks, glass, wood, metals, as well as more harmful components like asbestos. All this material is normally produced during construction and restorations, but this may include unfortunately also waste produced by catastrophic events like earthquake.

C&D waste is considered priority waste in European Union countries and it represents a major concern to recycle and re-use it for new applications and products. Recycling and utilization of such waste would be a significant contribution to the environment and sustainable development towards the adoption of "zero waste" principle. Currently, in Italy, 75% of CDW is being recycled, roughly twice the average percentage among the EU members because many show no confidence in the composition and quality of CDW-based products.

The vitrification of C&D waste may represent a valid and useful technique to thermal treat such materials in order to increase significantly the possibility of reutilization, which at the moment is still limited as a low-grade filling aggregate use (REF). For this reason, in this study we have investigated the possibility to obtain glass and glass-ceramics materials from C&W waste and C&D waste mixed with different types of material, as for example recycled glasses, fly ash, bottom ash and tile cutting slag. To attain so we have performed vitrification experiments at lab scale in a muffle furnace at ambient pressure, temperature ranging from 1000 to 1200 °C and different melting duration (2-16 h). The obtained materials were investigated by means of different analysis, by using at first optical microscope, powder X-ray diffraction (XRD) and scanning electron microscopy (SEM). At the end feasibility of industrial production of new type green building material is discussed in order to achieve waste recycle and environment protection.

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"Trap Efficiency" loss of artificial reservoirs through a direct and indirect evaluation of soil erosion rate in a sample catchment of Central Italy.

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Sediment is an essential, integral and dynamic part of a river basin, cause a healthy river needs sediment as a source of life. On the other hand, the abundance of sediments can act as a potential sink for many hazardous chemicals and, especially in the case of artificial reservoirs, produce a long-term loss of storage capacity for reservoir operation and watershed management.

Even the European Water Framework Directive (WFD), although it does not deal specifically with sediments, clearly identify a link between sediment monitoring in a river catchment and the achievement of the WFD objective itself (good status of all European water resources by the year 2015). The study, using different direct and indirect methodologies, wants to evaluate the sedimentation rate within a sample artificial reservoir (Le Grazie lake in central Italy) which, in the period 1952-2015, has caused a strong decreasing of the trap efficiency and a loss of over 70% of the water volume stored. Direct measurements of the lake bottom bathymetry, carried out in 2006 and 2015 (AGEOTEC, GEOMARINE), and 3D reconstructions performed in a GIS environment, made it possible to calculate volume and weight of filling material and, in particular, to verify that the greatest contribution comes from a right tributary of the Chienti river (the San Rocco stream), deepened in a clayey subbasin, and flowing directly into the lake. The values obtained have been then compared with those coming from indirect evaluations carried out using the RUSLE (Revised Universal Soil Loss Equation) Method (Wischmeier and Smith, 1982) performed in the San Rocco subbasin. The comparison between the two approaches made it possible to compensate for errors inherent the methods themselves (uncertainties in the direct measurements or the parameters used in the RUSLE equations) and, above all, to verify an upward trend in the sedimentation rate starting since 2006.

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Numerical viscoelastic modelling of rifting processes

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We describe the geodynamic evolution of a rift through a 2D thermo-mechanical numerical model based on a non-linear anelastic rheology and physically consistent boundary conditions. The model has the objective to test the possibility that the lithosphere retains some amount of elastic strain energy during the rifting phase, which will be subsequently released after the onset of sea floor spreading by anelastic relaxation. Our tests were performed using Underworld II, an open-access Python geodynamic code, and 'open' boundary conditions. An alternative simpler numerical model with 'closed' boundary conditions was also considered to evaluate the influence of small-scale convection on the rifting process. Our results show that the model of rift-drift transition proposed by (1) and (2) is supported by a realistic pre-drift evolution of the lithosphere.

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A new methodological approach through the LCA procedure for the evaluation of a massive limestone quarry.

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Life Cycle Assessment (LCA) is a methodology used to quantify potential environmental impacts of the entire life cycle of a product or service, starting at raw material acquisition, following with production, use, and eventually its disposal. Today, LCA is used for sustainability benchmarks or comparisons of products in the framework of investment decision, product development or even engaging subcontractors. More recently, the EC elected LCA as the method to calculate environmental indicators for comparisons between products and organizations. LCA is a crucial part of the transition to a green economy, and the privileged method for calculations of environmental impacts. The purpose of this work is to quantify and evaluate the environmental and energy performance (materials used in the processing), resulting from the entire life cycle of the micronized limestone, as well as comprehend the life stages of the production process. The project, which aims to harmoniously combine the industrial needs of the existing mining activities, with the respect of an area particularly sensitive from the environmental point of view, is focused on the extraction of limestone from the formation of the Massive Limestone (Upper Triassic) with a content in CaCO3 more than 98%. Since a few years the mine has developed innovative techniques to reduce the environmental impacts of its activity, such as the underground cultivation method, that involves the creation of 8 underground large chambers, inside the mountain.

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Thermophysical parameters from laboratory measurements and in-situ tests in borehole heat exchangers

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Laboratory and in-situ tests were carried out with the aim of investigating underground thermal properties and mechanisms of heat transfer of a pilot ground-source heat pump system consisting of two borehole heat exchangers. Samples of grouts used for filling the boreholes and of the main lithotypes penetrated by drilling were analysed in the lab for assessing their thermal properties. Grouts with different mechanical characteristics and similar mineral composition were used in the two holes. The grout thermal conductivity ranged from 1.65 to 2.13 W m^{-1} K^{-1} and thermal diffusivity from 0.61 to 0.80 μm^2 s^{-1}. Thermophysical measurements on the lithotypes showed the largest thermal conductivities (2.34-2.66 W $m^{-1}K^{-1}$) in sandstones and marls, whereas pelitic lithotypes denote lower values (1.82-2.21 W m^{-1} K^{-1}). The average thermal diffusivity was 0.73 Î¼m2 s-1. The *in-situ* experiments included thermal logs, to evaluate the undisturbed underground temperature, and thermal response tests, which were interpreted with the moving line-source model to infer the underground thermal conductivity, the borehole thermal resistance and the groundwater velocity. The inferred thermal conductivity varied from 2.09 to 2.48 W m^{-1} K^{-1} and thermal resistance from 0.188 to 0.192 m K^{-1} W^{-1}. Values of Darcy velocity ranged from 5 to 9*10-7 m s-1. After the heat injection tests, the temperature variation with time was recorded at 20-m-depth intervals in both holes. The temperature-time series were used to assess the thermal conductivity variation with depth. In both boreholes, thermal conductivity was little variable from 20 to 80 m depth (2.14-2.34 W m-1 K-1) and it increased (2.49-2.68 W m^{-1} K^{-1}) at the hole bottom. The average thermal conductivity for the two boreholes was quite similar (2.29-2.32 W m^{-1} K^{-1}) and consistent with the values obtained with the moving line-source model. The results obtained with this approach were also consistent with the laboratory measurements and gave estimates of thermal conductivity at different depths.

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Fault-Related Geothermal System: an Example from the Tocomar Basin (Central Puna, NW, Argentina)

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A new conceptual model for the Tocomar Geothermal System (TGS) based on geological, structural and geochemical data along with the available geophysical data is presented. The outlining of conceptual models, even in the earliest stages, represents a paramount aspect for geothermal exploration since these schemes are by far the most effective cost-benefit tool. In fact, reconstructing stratigraphic and structural framework is fundamental for i) understanding the relationship among cap rocks, reservoirs and fluid circulation, ii) geothermal potential, and iii) planning resource exploitation. The TGS is located in the Central Puna (Central Andes, NW Argentina), related to the 0.57 Ma Tocomar volcanic center (TVC) emplaced in a small extensional basin "Tocomar basin (TB)" linked to the active NW-SE trans-Andean tectonic lineament known as Calama-Olacapato-Toro (COT) fault system. The pre-basin succession is made of low-grade metamorphic and sedimentary lower Paleozoic rocks, Cretaceous continental rift-related deposits and ignimbrites from the Aguas Calientes Caldera (10-17 Ma). The basin infill consists of a thick alluvial deposit formed by polymictic conglomerates and sandstones that evolve upwards to several pyroclastic deposits. The updated conceptual model for the TGS consists of a heat source related to the 0.57 Ma rhyolitic magmatic activity of the TVC. The geothermal reservoir has a NW-SE geometry elongated along the COT-like Chorrillos fault, with a minimum area of ca. 6 km2. The average depth of the top of the reservoir is 1,000-1,400 mbgs, probably hosted in Cretaceous sedimentary rocks. The primary permeability is enhanced by intense deformation along the COT. Both the interbedded fine-grained Cretaceous facies and a hydrothermal clay cap (argillic alteration) act as seal rocks. Hot springs occur in association with deep N30-N60 fractures related to the COT. Temperature estimation using the NA-K geothermometer indicates reservoir temperatures of 184-230°C. Estimated local geothermal gradient for the TB is 150 °C/km and the minimum stored heat in the geothermal reservoir is of about 3.21x1015 kJ.

Gravity-driven processes in the near-platform basinal carbonates: A case study from Gargano, Southern Italy.

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Gravity-driven processes, such as sliding, slumping, debris-flows and creep, can have a significant impact on the evolution and the architecture of the platform-to-basin carbonates. The distribution and nature of mass-wasting products and related features can affect the fluid flow migration pathways, and lead to unexpected compartmentalization issues in reservoir analysis.

A structural and sedimentological analysis was performed in the eastern margin of the Cretaceous Apulian Carbonate Platform in the Gargano Promontory, southeast Italy. Here, subseismic-scale mass-transport deposits (MTDs) comprise a large proportion of basinal Maiolica Formation. These MTDs typically display a vertically bipartite character, including debrites and slump deposits of varying volume ratios. The slumps are composed of the beds of surrounding formation, meanwhile the debrites are composed of clasts of slope provenance. Some confined packages composed of folded beds display bent stylolites with radially oriented peaks at the bedding interface which infers post-lithification folding.

The succession is cut by both tectonically- and gravity-related faults of small to large scale. The gravity-related (superficial) faults are mostly normal, and their strike is consistent with the strike of the paleoslope. This demonstrate an extensional regime and downslope movement. The succession bisected by superficial faults is likewise cut by discordant large-vertical breccia bodies. The breccias reaching up to 80 m of height and 40 m of width, are mostly chaotic in nature and several of them were influenced by dolomitization. These breccias are most likely the products of downslope extension. Studied features at the outcrop scale and previous existing studies from the sub-surface, enabled the construction a conceptual model of superficial and deep-seated gravity-driven features and their impact on the paleoslope-to-basinal carbonates.

LandscApp: a medium to connect Society to Geoheritage

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Landscape is so relevant in the culture and economy of our country, that it is clear how important can be the knowledge of its geomorphologic characteristics and natural history as well. Highly significant is the sharing of such knowledge: a mandatory step to involve local communities in those actions oriented to a balanced management of the territory, to the protection of those environmental, aesthetic and cultural resources, characterizing our Country and to the creation of opportunities for social/economic promotion as well. Different needs in knowledge suggest new strategies, and dialogic interaction between researchers, policy makers, stakeholders and society in order to offer the public an opportunity to experiment with an alternative and conscious approach to the rich natural and cultural heritage of the territory, using new tools, synthetic and complete, suitable for all levels of users.

LandscApp is a new App containing information on the geomorphological and environmental settings of the Italian Landscapes, related to some social themes significantly linked to the territory. Moreover, referring to the vocation of some areas to outdoor sports, the App contains information and news related to the most significant performances realized by the most famous champions of skiing, cycling, hiking, climbing, in the magnificent natural scenery that characterize our country. Non-conventional scientific communication takes on a strategic importance today, particularly referring to the knowledge of the territory, and to rerritorial planning, risk prevention and sustainable development. To this aim, GIS and 3D modeling are flexible and friendly tools, useful both in educational plans and in territorial promotion, suitable to communicate Environment, Landscape, Territory to a wide audience. In this regard, we suggest a creative combination of landscapes, food and wine, tourism and sport, a new integrated field that could stimulate actions to promote sustainable development in Italy, within a more sensible culture of land use. A first version of the App ia available online: www.ost.sinanet.isprambiente.it/.

It was created for the Ampezzo Dolomites, an area representing -for its beauty, its significance and the amount of documentation available- the ideal 'ontext to develop and test an appropriate methodology, creating a reference prototype. Landscapp has been presented in Cortina d'Ampezzo, at the Ciasa de ra Regoles, guest star and testimonial the ski 90's champion Kristian Ghedina.

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Learning Sciences through Gaming

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The GeoQuest Project started as a PhD research project in Teaching and Learning Processes in Geoscience Education at UNICAM. It aims to answer to both students and teachers'needs in an ever-changing world. Today, in particular, students need teaching tools that use different communication codes, as they are less accustomed to abstraction. An increasingly interconnected and technological world requires students to have specific skills: knowledge of the disciplines founding cores in an interdisciplinary key is required, along with technical and technological skills, mastery of foreign languages, flexibility, attitude to team working, creativity and entrepreneurship. Scientific subjects, such as Science, Technology, Engineering and Mathematics (STEM subjects) need to be strengthened and studied through a laboratory approach. On the other hand, teachers need user-friendly teaching tools, which allow and promote teamwork, which allow the laboratory teaching and the CLIL (Content and Language Integrated learning) approach.

We have therefore developed a Computer Classroom Role Playing Game (CCRPG), GeoQuest, which has been object of a multi-phase experimentation carried out for two years in Italian school of different grades.

The final outcome of the GeoQuest Project is that the game effectively matches the needs identified by students and teachers. Carrying out the experimentation in several phases allowed us to calibrate and improve our project and allowed us to obtain rigorous and reliable results. This allows us to assert that we have been able to meet the needs of students and teachers, with a teaching tool that perfectly complies with the demands of modern society. Above all, our project answers our research questions in teaching and learning processes in Science Education: to create an educational tool that ensures students build knowledge of the disciplines founding cores in an interdisciplinary key, which allows them acquire technical and technological skills, mastery of foreign languages, flexibility, creativity and entrepreneurship.

Waste Material Based "Terrazzo" Tiles: The Effect Of Curing Time And Extreme EnvironmentalConditions Over Glass Aggregate/Cement Matrix Boundary

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Currently, more than half of all materials extracted globally (over three billion tonnes/year in the EU only) are transformed for use in construction. Before year 2020, the EU aims to reduce the environmental impact of the construction sector by recycling or re-using large amounts of these materials, thus reducing the consumption of raw materials and helping promote the sector's economic stability. With this challenge in mind an aesthetically pleasant and fully recycled (up to 78%) pre-cast cement based tile (Terrazzo tiles) was designed by replacing raw materials with Glass Waste (GW) and Construction/Demolition Waste (CDW). Several recent studies explored the effect of the addition of GW in the manufacture of urban pavements, concluding that the use of GW can improve various phases of pavement life and structure by enhancing the structural performance, durability, environmental friendliness, and aesthetic features.

In this study we extend this knowledge also to interior cement-based tiles by evaluating the technical performances of this this novel designed tile, in particular by focusing on the interface between the GW aggregates and different Portland cement based matrix at extreme environmental conditions. For this work three representative waste material based "terrazzo" tiles were selected and characterized by means of XRD and SEM imaging in order to study the boundary effect between GW aggregate and different binding materials: limestone powder, quartz powder and fine ground WG powder. A fourth additional mixture of Portland cement and CDW material was characterized. Fragments of a Limestone matrix tile were also thermally threated at -18°C and at 60°C for one week to witness the possible formation of new harmful phases at the grain-matrix boundary.

Preliminary results on X-ray diffraction patterns show that 1 year after manufacture and/or thermal treatment there is no new formation of harmful phases other than the starting ones. High magnification SEM imaging further confirmed this observation also highlighting the good binding performances of a mixture composed by the 78% of recycled WG.

Magnetic and radar prospections at the World's heritage Hadrian's Villa

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A combined magnetic-radar survey has been performed in 2017-2018 in the area surrounding the Hadrian's Villa Plutonium, near the city of Tivoli, Italy. The objective was to detect buried buildings and delineate the local structure of the underground system of tunnels that links different areas of the Hadrian's Villa. We show that several buried structures are present around the exposed part of this monumental building. The new geophysical data also show that a complex system of interconnected tunnels of different size exists in this area. The radar survey was performed using a GSSI SIR 4000 system equipped with a 200 MHz antenna with a maximum penetration depth of 9 m. This antenna allowed to obtain sufficient penetration for investigating the system of tunnels that were dug in the tuff units underlying the Plutonium-Inferi area, although with a lower resolution relative to a 400 MHz antenna. However, due to the particular chemical and physical properties of the soil and tuff units in this area (e.g., a very high magnetic permeability), we obtained a depth of penetration not exceeding 4 m. We compiled three depth slices, corresponding to the following depths intervals: 30-80 cm, 80-130 cm, and 130-220 cm. Total field magnetic data were collected on a terrain clearance using a Geometrics G-858 caesium vapor magnetometer. The magnetic data were read at 10 Hz along bi-directional survey lines equally spaced 0.5 m. All the total field measurements were performed in solar-quiet conditions, with a Kp index not exceeding 2. The data were corrected for the daily variations of the geomagnetic field through a levelling procedure and underwent standard pre-processing consisting into despiking and decorrugation procedures. The GPR and magnetic data were supplemented by two electric resistivity tomography (ERT) profiles, which were acquired to assess the presence of tunnels. The last series of data consisted into 9 tuff cores sampled from the tuff unit beneath the Plutonium area and from some soil samples. The cores were analyzed at the ISMAR-CNR paleomagnetic lab of Bologna with the objective to determine the magnetic parameters of these rocks and soil samples. Both these data will be used in the magnetic modelling of the buried structures and cavities (1,2,3).

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Magnetic and radar prospections at the Roman fortified military camp of Paleokastër, southern Albania

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We report on a combined magnetic-GPR survey performed in July 2018 at a Roman castrum located 10 km north of Gjirokaster (Albania), close to the village of Paleokastër. The fortress is situated on a low promontory of alluvial deposits formed by the confluence of the Drinos and Kardhiq rivers, dominating the main north-south route through the province. Baçe (1) suggested that it was constructed in the early fourth century. Shortly afterwards it was destroyed during the Gothic incursion of 378 AD. The fortress was converted into a Byzantine civilian settlement during the fifth and sixth centuries. During this period, two Christian churches were constructed, one inside and one outside the walls. Magnetic and GPR surveys were carried out at Paleokaster, in order to determine the arrangement of buried structures and reconstruct the archaeological history of this settlement. Magnetic data were collected in gradiometer configuration using a Geometrics G-858 caesium vapor magnetometer. We generated both vertical gradient and total field anomaly maps. The latter were produced with the objective to build a magnetization model of the buried structures using a forward modelling approach (2, 3, 4). Radar surveys were carried out using a GSSI SIR-4000 system equipped with a 400 MHz central-frequency antenna.The filtered radar profiles were then processed to produce horizontal amplitude slice maps and 3D isosurfaces. The collected data consistently revealed the existence of Roman age buildings within the fortress, for example headquarters at the crossing between the vie pretoria and principalis and other alignments corresponding to the soldier barracks. We also detected structures laying beneath the Byzantine church, most likely assiciated with the previous Roman seattlement. The general arrangement of the shallow structures shows the typical military organization of a Roman castrum, with the overprint of Byzantine buildings, although some enigmatic deeper structures, possibly of Hellenistic age, are revealed by the analysis of the amplitude slices.

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New heights in the digital geology revolution: using UAV-based aerial imagery and 3D digital outcrop models and changing geologic field methods

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Over the past decade, field geology has experienced a digital revolution spurring new methods for rapid data acquisition and enhanced analytic capability leading to fully digital geologic maps and visualizations. During just the past several years, a surge of accessible and affordable UAV aerial platforms allow field researchers to reach new heights gaining perspective on outcrops and geologic scenes never-before accessible.

By integrating UAV-acquired aerial imagery data sets using Structure from Motion (SfM) photogrammetry, geologists have the ability to build 3-dimensional georeferenced digital outcrop models (DOM) of objects large and small. SfM data returns come as 3D point clouds and solid surface reconstructions that compete with airborne and terrestrial laserderived (Lidar) data sets which are often cost-prohibitive and lack the operational flexibility needed to solve some geologic issues. Commercial-grade UAVS, however, provide a costefficient solution that can be flown in a wide array of circumstances to gain the proper elevation and range to acquire ground surface heights, vertical outcrop data. and orbital surface scanning to acquire the necessary coverage of 3D objects.

We here present a suite of 3D digital outcrop models from several active research locations by the Unicam Geology Division Reservoir Characterization Project to illustrate the utility, effectiveness, and versatility of this new approach across geoscience. The featured sites include faulted deepwater clastic depositional systems, submarine mass transport complexes, and shallow water carbonate facies. These DOMs serve not only as pretty pictures but rather as volumes of quantitative outcrop data and the basis to measure and acquire geologic data and build interpretations. This method not only expands the view of a field geologist but supplies enormous amounts of data that would otherwise take several weeks of field mapping to collect.

The impact of mechanical stratigraphy on fracture propagation in heterolithic siliciclastic beds in below seismic to seismic scale faults

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Heterolithic beds in siliciclastic rocks provide a unique opportunity to study fracture propagation and growth in mechanically different stratigraphic layers that undergo the same structural deformation. Fracture distribution and lithology plays a significant role in fluid flow. Although only faults > 15 m are visible in seismic images, fluid flow in below seismic scale resolution faults are imperative when correctly predicting the productivity of a natural reservoir. In order to accurately model subsurface reservoirs, one needs a comprehensive understanding of the effects of below seismic faults that are present in a fault system.

For this study, we have chosen two formations: 1) the Miocene Cilento group, located in southern Italy in the Campania Region and 2) the Miocene Macigno formation, which outcrops in southern Tuscany. The Cilento group outcrops near the coast of the Tyrrhenian sea and into the internal mountains. Here, the outcrops are made up of sandstone-pelitic and marly-calcarenite turbidites, with conglomerate intervals that are generally deposited unevenly throughout the section in thin and medium layers.The Macigno outcrops between the towns of Livorno and Piombino. It is represented by foredeep siliciclastic succession dominated by turbiditic sandstones with minor siltstones, mudstones, and shales that are evenly distributed throughout the section. With these two study areas, we can study faults from initial nucleation to well-developed fault systems in both evenly and unevenly distributed heterolithic beds, that have undergone similar deformation phases. By comparing these two types of heterolithic beds, we can study the how different mechanical properties in differently distributed beds effects fracture nucleation and propagation in small (0 - 5 m), medium (5.1 - 15 m), and large (15.1+ m) faults.

Evaluation of rough surface's parameters and fluid flow properties

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The full description of rough surfaces of fractures and their apertures is a crucial step toward enhancing our concepts of the parameters which control fluid flow through rocks. The purpose of this study is to extract roughness properties of a natural rough rock surface by spectral analysis, and presents a new mechanism of opening fracture aperture , which assumes that hydrostatic pressure variations causes opening the fracture aperture by a tiny parallel displacement (less than 1% of length of fracture) to fracture surface. The main target of simulation is to investigate relation between the displacement, fractal dimension and permeability. By using Fourier power spectrum to analyzing fracture surface topography, that provides a reliable method to estimate roughness parameter 'fractal dimension' which is the main parameter controls the surface roughness. Form this parameter ' fractal dimension' will be used to generate synthetic fractures, those fractures will have the same fractal dimension value of the original one but with different parameters. Finally, a fluid flow simulation will be conducted to estimate values of permeability of natural fracture and these synthetic fractures to find a relation between parameters of surface's roughness (especially fractal dimension) and fluid flow properties.

Water in Pantelleritic glasses measured by FTIR and Raman spectroscopy

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Water is an important component for controlling volcanic eruption styles due to its influence on magma viscosity, liquidus temperatures and phase equilibria as well as the diffusivity of melt components. Thus, knowledge of water solubility in silicate melts, and how it varies with pressure (P), temperature (T), and melt composition (X) is of fundamental importance for understanding and quantitatively modelling common magmatic processes. There exist considerable H_2O solubility data for the most common magma compositions (e.g., basalt, calc-alkaline rhyolites) but data for more diverse compositions (e.g., phonolites, pantellerites/peralkaline rhyolites) are limited, even though considerable analytical data show such magmas may be quite H_2O-rich and capable of producing strongly explosive volcanic eruptions. In order to develop quantitative models of H_2O solubility for a wider range of P-T-X conditions, we have been conducting new experiments to measure H_2O solubility in peralkaline rhyolitic compositions, at P= 25-250 MPa, and T= 800-900°C. These data will be useful for better understand the pressure conditions of hydrous peralkaline magma storage and degassing dynamics during magma ascent. Our new H_2O solubility experiments on pantelleritic melts, concentrate mainly on the pressure and alkali (ratio Na/Na+K) effects. Initial results indicate that higher Na and pressure favour higher water solubility in these melts (Stabile et al., 2018) and solubilities on a wt% H_2O basis (from 50 to 200 MPa) are 40-50% higher compared with metaluminous rhyolitic melts.

To better characterize the water speciation in these glasses, Infrared and Raman Spectroscopy have been employed, with the aim of providing a calibration of IR/Raman measurements of water in pantelleritic glasses. This is essential because of the lack of such studies in literature. The preliminary results show that the extinction coefficients of both the 4500 - and the 5200-cm-1 bands (assigned to molecular water and hydroxyl groups, respectively) are significantly different from those for metaluminous rhyolitic glasses. These results will help to enlarge the dataset for alkali-rich and silica-rich melts and facilitate improved quantitative measurements of water in peralkaline glasses using FTIR and Raman spectroscopy.

Chemical and Mineralogical characterization of BA combustion products

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Among the different types of combustion output from Municipal Waste Incinerators (MWI), bottom ashes (BAs) are the primary form of solid products, typically representing 15% of the input waste mass; other less abundant waste products include fly ash (FA) and Air Pollution Control (APC) residues. The BA are inhomogeneous materials and consist mainly of poly-crystalline fragments, glass, silicate minerals, and metallic Fe, and lesser amounts of many volatile metals, e.g. As, Cd, Cr, Hg, Ni, Pb, Zn. In this study we have investigated two sets of BA samples derived from two incinerator facilities, one located in Rimini and the other in Piacenza. The main aim of the work was to mineralogically and chemically characterize the products prior to and after vitrification treatments carried out between 1000-1300°C in a 1 atm muffle furnace. Vitrification, among different techniques used to treat and homogenize waste products, is considered a valuable process to reduce waste volume and reduce hazardous element concentrations (Cl, S, volatile metals) for further re-utilization of the BA waste. Mineralogy is considered the main way to investigate the possible host phases for potentially hazardous elements in bottom ashes and, for this reason, a detailed mineralogical study of solid residue wastes has been carried out by using X-Ray Diffraction (XRD) analysis.

XRD scans show that the main phases present are silicates, oxides and carbonates and this is of interest for the characterization and reuse of bottom ash. In fact, high contents of stable silicates and oxides produce a positive effect whereas concentrations of sulfates and chlorides have a negative impact on their properties and possibilities to be applied in structural and civil engineering fields. Furthermore, XRD analyses confirm that the thermally treated samples are generally glasses (broad background bands from 17° to 38° of 2T; e.g. Bish and Post, 1989) with only small peaks corresponding to trace amounts of the refractory magnesio-ferrite phase. This is the only resistant mineral with high stability temperature (stable to 1665 °C, Ambruz et al., 1980) which may be found in the vitrification products.

The 2030 Agenda for sustainable development and consumption of the georesources: an interdisciplinary activity

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Starting from the theme of circular economy, emphasised in the 2030 Agenda[1], we developed a two hours didactic activity, carry out during in-service training for teachers (Summer school 2018 in UNICAM). The objective was to present an activity on Geomaterials and Georesources, topics usually neglected in the middle school programs (Fig. 1), as starting point for an interdisciplinary activity for the Environmental Education.

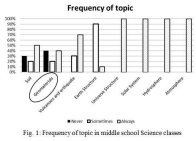

Fig. 1: Frequency of topic in middle school Science classes

Different wastes coming from packaging (glass, plastic, aluminum) were collected in order to focus teachers' attention to the use of georesources and the energy required for the production of a kg of waste. The Wasteberg[2] was then introduced, built using cardboard divided in two parts.


Fig. 2: Teachers at work

The upper part, smaller, containing some waste, the lower part, larger, empty. The lower part is supposed to be filled up with drops as symbols of what was produced, emitted or consumed (such as Soil, Water, CO_2, etc.) to produce the object glued in the upper part of the Wasteberg.

Then the IBSE question was proposed: *how much waste do I produce when I throw away 1 Kg of waste?* The question seems tricky but it actually encourages to think about resources consumption in the whole productive process. Teachers, in groups (Fig.2), were asked to integrate some interdisciplinary aspects with contents of math, history, geography and technology. The good results obtained from questionnaires (Fig.3) are an indication that this type of interdisciplinary activities are accepted with favor by the teachers which possibly will use them in their classes, using a new interdisciplinary approach for teaching Geosciences.

Fig. 3: Results from teachers' questionnaire (n=32)

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3d-Geological Model of the Superficial Faults Reactivated During the 2016 Central Italy Seismic Sequence

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The 2016 Central Italy earthquake sequence, consisted of three main shocks and thousands of secondary events, produced significant surface ruptures along the SW-dipping normal Mt. Vettore-Mt. Bove Fault System (VBFS).

The seismic sequence started on the 24 August with a Mw 6.0 mainshock located at 1km west of Accumoli village. After this event, ∽N155°-trending surface ruptures, mostly SW dip-slip kinematics, were recorded for several kilometers along the southern portion of the VBFS. Two months later (26 October), a new mainshock of Mw 5.9 occurred at 3 km NW of Castel Sant'Angelo sul Nera village, caused discontinuous ground ruptures along the northern portion of the VBFS. After 4 days (30 October) the largest shock of Mw=6.5 occurred close to the Norcia village. An almost continuous pattern of surface ruptures was observed for an overall length of 20-25 km along the whole VBFS, generally reactivating the 24 August and the 26 October 2016 ground ruptures. Surface rupture displacement exhibits normal dip-slip kinematics, with an average 0.5 m throw.

In this work we present a 3D geological model of the VBFS, powered by a former high geological and structural knowledge of the area and a robust database about coseismic fault reactivation (e.g. orientation, length, throw; Villani et al. 2018). Furthermore, a comparison of the geological and coseismic offset by means of length/displacement profiles has been carried out, leading to the retrodeformation of the three faulting events.

The aim of this study is (i) to characterize the highly fragmented surface ruptures observed after the Mw=6.5 seismic event in terms of fault dimensional parameters and (ii) to compare the long-and short-term deformation along the VBFS. The achieved results contribute to a better understanding of the existing relationship between superficial structures and deep seismogenic faults, with implication for the seismic hazard evaluation and related applications along the axial zone of the central Apennines.

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Mathematics

Optimal Output Regulation for Underactuated Systems

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Our research addresses the problem of optimizing the output regulation for underactuated systems, typical in the framework of autonomous robots, such as underwater vehicles and aerial vehicles. When a system is underactuated, only subsets of the outputs can be independently controlled. We investigate the problem of finding the input that minimize a cost function of the overall output tracking error, and how such solution is related to the inputs associated to the singularly optimal regulation of each output.

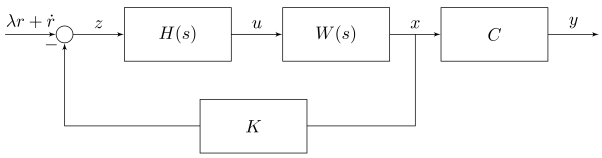

Figure 1: dynamic compensator H(s) in the closed-loop system

[1] and [2] are some preliminaries results to obtain the optimal open-loop controller for constant, periodic and quasiperiodic references in a single-input multi-output framework as a linear combination of singularly optimal controllers. In [3] the same approach has been applied to find the optimal closed-loop controller for constant references, while [4] extends the results in a multi-input, multi-output framework: while all the previous results use a linear combination of singular optimal controllers, this last work introduce a dynamic compensator to handle time-varying references with a closed-loop controller. In [5] we apply the same ideas to the more challenging context of LPV-systems.

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Self-balancing Electric Motorcycle Modelling and Control

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In the autonomous driving the main challenge is vehicle stabilization with electronic control systems - even when vehicle stops - which can enhance riders' safety. A mathematical model which captures its main dynamics is needed for control system design, but such models has not been thoroughly investigated at low speed without the use of the steering handlebar[1].

In the work a validated model of a two wheels drive electric motorcycle has been derived with the specific goal of a model simple but able to capture all the dynamics relevant to the capsize motion of two-wheeled vehicles. For these purposes, the work presents a 4 degrees of freedom model dynamically similar to an inverted pendulum that considers both rear and front wheel driving torques instead of rear driving torque and steering one as control inputs. Moreover, steering axis is initially set on a strictly positive steering angle and is constant over time. The study would also find out whether front wheel driving torque actuation with a rotated steering axis can help balancing when steering torque is not actuated. The analytical equations of motion are given by the Lagrangian approach: the result is a nonlinear second order ODE system in four unknowns - roll and yaw angles and rear contact point coordinates.

The mathematical model has been then validated by FastBike, a computer simulation multibody software for dynamic analysis of two wheeled vehicles which includes five bodies, a nonlinear tyre model and nine degrees of freedom. The software has been suitably modified for low speed range. In validation process a sliding mode control strategy has been designed using the analytical model and then applied to the multibody one[2]: the simulations show a good match in roll and yaw angles comparisons. This indicates that the mathematical model captures the main dynamics and can be used for model-based control design.

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Euclidean method and epistemology in the works of Giacomo Leopardi

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Giacomo Leopardi (Recanati, 1798 - Naples 1837) has been one of the major writers and thinkers of the early 19th century. Exceptionally talented, in his youth he studied, in addition to Italian, Latin and Greek grammar and metre, exact and experimental sciences. In particular, he deeply absorbed the Euclidean method and wrote short essays (Dissertazioni) concerning all the most relevant aspects of theoretical and experimental physics known at his times[1]. It is proposed herein that the scientific reasoning acquired in his youth has contributed decisively to the philosophic thought of Leopardi, as it led the author to a profound epistemological awareness. Thanks to this, Leopardi was able to produce sound assessments of the scientific novelties of his age, which included the discovery of new galaxies, findings of fossils of prehistoric animals and the alleged observation of artefacts on the lunar surface. Moreover Leopardi, in his Zibaldone (an ample collection of personal thoughts, used as a framework for the artistic production) made bold statements on a number of open scientific questions, such as the possible existence of universes where Newton's law is not verified, a scenario in which the universe undergoes an indefinite sequence of collapses and rebirths, the nature of the differences between human beings and other animals. Finally, an aspect deserving particular attention concerns the epistemology of music, conceived by Leopardi as a phenomenon which pertains not to Nature, but to a "second nature", which springs from the coupling of some basic acoustic elements with the cultural "addictions" of each given epoch. This point of view, elaborated in the Zibaldone, turns out to be very fruitful in order to conceive of harmonic science as a modeling, even in a mathematical sense, of musical phenomena, without reducing them to psycho-physical data out of history. It consequently proves particularly useful for understanding the role of music in the relationship between ancient and modern science[2].

In conclusion, the reconstruction of the epistemological thought of Leopardi offers a precious occasion for rethinking the concept of unity of culture from a methodological as well as didactical point of view[3].

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The model theory of modules over Bézout domains

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Model theory is a, comparatively young, branch of Mathematical Logic but is already able to provide new and fertile methods and tools to other parts of Mathematics, for example Algebra and Algebraic Geometry, in particular in the theory of modules over a given ring. This is the wider setting we are interested in, and we focus on modules over Bézout domains, more generally over Prüfer domains - a class of rings rich in important examples. On this topic we collaborated with G. Puninski (who died untimely one year ago), and we are still working with F. Point (Mons-Paris Diderot). The model theory of modules over Bézout domains is developed in 6). Several papers are devoted to decidability of theories of modules over such rings and many give a related description of the Ziegler spectrum of the underlying ring. This is done in 5) and then more generally in 1) over valuation domains, in 7) over Bézout domains obtained via the so called D+M construction, in 4) over the ring of algebraic integers and, finally, in 2) over arbitrary Bézout domains (and indeed Prüfer domains) with infinite residue fields. The finite residue fields case is work in progress. Let us also mention 3) for a complete analysis of the Ziegler spectrum over the ring of complex valued entire functions (where the decision problem makes no sense). See 8) for an extended report on the whole matter.

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Literature review toward decentralized railway traffic management

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This paper addresses the analysis of the state of the art on the use of artificial intelligence to tackle problems which may help in designing a decentralized railway traffic management system. Today's approach to traffic management is the imposition of the centralized decisions made by an infrastructure manager on trains' routing and scheduling in case of perturbation. As a change of paradigm, we are interested in decentralizing this decision making having trains autonomously reaching an agreement on their interactions. Thus, the goal is the study of new ways for modelling rail traffic based on the idea of multi-agent systems. Initially, we discuss the possibility of using the existing research works on driving agents in road traffic as a basis. The analysis of these works clarifies that the road traffic problems tackled with multiagent systems in the literature are not the same as the one we are interested in for railway. Specifically, major differences exist in the need for collaboration and agreement in general. Hence, we focus on the more general literature concerning these needs in multi-agent systems, and in particular on three different decision making approaches. First, we analyse the rich literature on consensus problems. Then, we study the problem of reaching a common decision in decentralized systems in general using the approach of hierarchical self-organization. Finally, we consider the possibility of applying task allocation techniques. After this overview, we propose a brief analysis on further possible research directions, which may drive the design of promising models for decentralized railway traffic management.

Keywords: Railway traffic management, Multi-agent system, Consensus problem, Hierarchical self-organization, Task allocation.

Development of a Wearable Device for Sign Language Translation

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Our study is addressed to develop a wearable device for sign language translation for the deaf-hearing support in ordinary life. Despite several studies occurred in the last decades, nowadays there is not a commercial sign language translation system that could improve the deaf-hearing interaction. In literature there are systems that use cameras for data acquisition (e.g.[1],[2] and [3]), but they lack of portability. For this reason, other systems are designed for gesture data acquisition, such as the data glove. A data-glove is a glove with sensors capable to give information about position, velocity, acceleration and orientation of hand, arm, shoulder and fingers or some of them.

Talking Hands set

The preliminary results of our research are presented in [5], where a prototype, called "Talking Hands". The different challenges have been overcame with simple solutions, since the main goal is an user-based product. Even if a satisfying communication experience can be offered to the final user, the actual solution can not handle with dynamic gestures, and the future research is addressed to solve this problem, without penalizing the usability of the whole system.

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Multivariate Garch Models for Wind Speed Time-Series Modelling

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Our work consists on evaluates the application of a family of VAR-mGARCH (multivariate GARCH) volatility models, especially a VAR-DCC model with Student's t innovations, to the problem of modeling (i.e. generating scenarios) and forecasting three univariate but mutually dependent wind speed hourly series, keeping into account that optimal modeling and optimal forecasting are not necessarily attained by the same models and that they are assessed by different types of metrics. This VAR-mGARCH family, originated in Finance, includes the VAR-BEKK model besides the VAR-DCC model, the latter seen as the simplified and more scalable version of the former. The models of the family are compared to two benchmark model sets, the first set consisting of three independent univariate Gaussian AR-GARCH models, the second set consisting of an individual Gaussian VAR model without GARCH sector. In order to highlight the usefulness of choosing coupled volatility schemes for modeling and forecasting spatially and temporally varying wind speed data, a controlled variance electricity generation portfolio example of Markowitz type, typical of Energy Finance, is also discussed at some length.

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Analytical Models to Validate the Mechanical Properties of Green Composite Materials for Wind Turbine Blades

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This work presents an analytical study aiming to predict the load history of a low-velocity/large-mass impact on natural fiber reinforced composite plates in view of a final application in the design of well performing wind turbine blades. Over the last decades, composites have become one of the most intensively used materials in many industrial applications. However, these materials show heavy limitations, such as low availability in the environment, non-biodegradability, and high fabrication costs. Therefore, natural fibers (e.g. flax, hemp, jute) might represent valid candidates to substitute synthetic ones (e.g. carbon, glass), being able to provide good mechanical properties while maintaining low production costs[1–3]. Since natural fibers have not been widely investigated from the analytical point of view yet, the proposed approach represents a valid tool to furnish a preliminary evaluation about the mechanical strength of green composites when subjected to a low-velocity impact. Both static and dynamic models previously introduced in the literature[4,5] are here adapted and validated when applied to hemp/vinylester composite plates, aiming to predict a threshold impact load for the damage onset and extent, and to draw an approximation of the load displacement curve. Compared to previously conducted experimental tests, the obtained analytical data demonstrate to be consistent and allow to predict useful information while saving costs and times characterizing an experimental campaign.

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Mathematics and Literature. Words, formulas, emotions

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We deepen the relationship between mathematics and literature, not only the search for positive or negative quotations on mathematics in literary masterpieces, but above all the analysis of a cultural bond rooted since the beginning of human culture: so Mathematics as language and creativity, and poetry or prose as a calculation. “Archimedes was as endowed with as much imagination as Homer”, writes Voltaire in his Philosophical Dictionary. This research perspective is strictly linked to teaching, within the so-called "Liceo Matematico (“Mathematical High School” national project, aimed at promoting the unity of culture. The collaborations include Gabriele Lolli (formerly SNS Pisa), Paolo Zellini (Rome 2), Paolo Maroscia (La Sapienza Rome), Paolo Pagli (Siena), and again Carlo Casolo (Florence), Claudio Citrini (Milan Polytechnic), Gian Italo Bischi (Urbino), Agnese Telloni (Politecnica Marche), and so on, plus other colleagues of Literature, such as Andrea Battistini and Paola Italia (Bologna), Giulio Ferroni (La Sapienza Rome), Lucia Perrone (Salerno) and many others. The project was developed in 4 annual meetings held in Salerno, organized with Paolo Maroscia, Saverio Tortoriello and Gianni Vincenzi and addressed to high school teachers and students. The contributions to the first two meetings are collected in 1) and 2) respectively. The references from 3) onwards regard the papers of the Camerino group.

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Physics

Development of an audio-frequency band vacuum squeezer for the quantum noise reduction in the Gravitational Wave detector Advanced Virgo

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Quantum Noise (QN) is one of the most important noise sources in the advanced interferometric Gravitational Wave detectors. In the previous interferometer generation the most relevant QN component was the shot noise, dominating in the high frequency region (300 Hz-10 kHz) of the detection band. The adopted solution to improve the sensitivity is to increase the input laser power up to 125 W. This high circulating power induces thermal effects, such as optical aberrations and parametric instabilities. An alternative solution, that would allow avoiding these drawbacks, consists into the injection of squeezed vacuum through the interferometer output port. The GEO Collaboration and the LIGO Scientific Collaboration already demonstrated a first sensitivity enhancement of their detectors using audio-frequency band squeezing. Now the Virgo Scientific Collaboration is working to implement this technique in Advanced Virgo. A facility for the production of squeezed vacuum in the audio-frequency band is being developed and preliminary measurements have been performed. This facility represents a first step toward new squeezing technique generation, also aimed at decreasing the radiation pressure noise, the QN component that would dominate when the other noise sources, that now limit the sensitivity in the low frequency detection band, will be reduced.

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In-situ XAS study of carbon-coated $ZnFe_2O_4$ anode material for lithium-ion batteries

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In this work we studied the structural and electronic structure (oxidation state) evolution of carbon-coated $ZnFe_2O_4$ nano-particles (ZFO-C) used as anode material in Li-ion batteries upon lithiation and delithiation by X-ray absorption spectroscopy at Fe and Zn K-edges. Previous works [1,2] have already shown that such material provides remarkable electrochemical performances (specific capacity higher than 1000 mAg^{-1} and high rate performance upon long-term testing) exploiting both alloying and conversion lithiation mechanisms [3]. However, the definite structural composition in the lithiated and de-lithiated state was not yet fully understood due to a general amorphization and formation of nano-sized crystallites [4].

X-ray absorption spectroscopy (XAS) is a suitable technique to investigate the local atomic environment and the oxidation state around Zn and Fe atoms. This technique has already been used at the As K-edge to study the evolution of the solid electrolyte interphase in the same anode material [5]. XAS measurements have been performed at ESRF for both Fe and Zn K-edge. The spectra have been collected in transmission mode using standard pouch cells for in-situ measurements and a set of ex-situ electrodes on carbon paper current collector sealed in PE foil at different stages of charge and discharge for comparison. The study of the XANES joined to ab-initio EXAFS simulations allowed us to get detailed information about the local structure, coordination number, oxidation state and variation of chemical environment.

During lithiation ZFO-C showed different behaviors. In the initial phase lithium ions insert into the spinel structure, stretching the cell and permanently inverting the spinel, swapping of half of the iron atoms in tetrahedral sites with zinc atoms in the octahedral ones. Subsequently, in the voltage plateau, we have a change of the oxidation states of iron and zinc, with the reduction of ZFO into Fe^{2+} and Zn^{2+} in a rock-salt phase metal oxide, as proposed by Bresser et al. [1]. Finally, those metallize and aggregate into metallic nanoparticles dispersed in a matrix of amorphous Li_2O. A further increase of capacity is given by the alloying reaction between lithium and zinc. In the de-lithiation phase iron gradually oxidizes and at the end of the process we obtain a mixture of Fe^{2+}, Fe^{3+} with residuals of metallic iron. Likewise also zinc shows the same trend presenting fractions of ZnO and metallic zinc.

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Design of a questionnaire to investigate high school students'conceptions about Cosmology and Universe

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As part of our ongoing research about the development of teaching-learning sequences (TLSs) [1] about astronomical phenomena [2-4], we focus on Cosmology and Universe (U&C) as meaningful contexts to teach up-to-date physics topics as nuclear reactions, light spectra, redshift and dark matter. We chose this subject because it is, at the same time, a fascinating topic and a content area where even university students frequently hold a variety of alternative conceptions. Previous research studies indicate that the majority of students (about 70%) is unaware that the universe is expanding [5-7] and believes that matter, as we know it, existed also before the Big Bang [6]. In some cases, students struggle to read and correctly interpret the Hertzsprung-Russell and Hubble's plots or confuse a galaxy with the solar system [8,9].

This study is guided by the following research question (RQ): *What is the students' pre-instructional knowledge about U&C?* To answer this RQ we have been designing a new questionnaire to assess students' conceptions about U&C.

On the basis of previous studies, we have developed a first draft of the questionnaire with open-ended questions. Twenty questions were conceived to target the following six key ideas in cosmology [9]: 1) Big Bang theory; 2) evolution, expansion and age of the Universe; 3) composition of the Universe; 4) time and distance scales for the Universe; 5) stars and galaxies; 6) dark energy and matter. The content validity of the questions was checked with two professional astrophysicists. We piloted the questionnaire with about 118 high school students (16-19 years) attending extra-curricular activities at our department about advanced physics topics. To score the students' answers we resort to a well established method. First, we developed an initial rating rubric with three levels: correct; partial and incorrect answer. Then we investigated the reliability of our findings through inter-rater agreement.

Emblematic students' answers will be used to design suitable answer choices for a multiple-choice version of our questionnaire. Students' answers to the multiple-choice answers questions will be then analyzed using Rasch analysis. Our aim is to assess whether the hypothesized key ideas form a coherent set of constructs that consistently describe students' understanding of U&C. Results will also inform teaching at undergraduate level and the development of suitable research-based TLSs at secondary school level about the addressed topics.

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Quantitative layer identification of two-dimensional Materials

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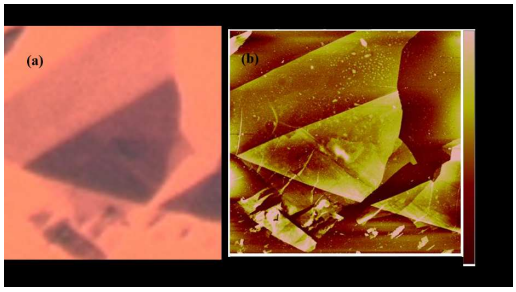
After the discovery of graphene, two-dimensional (2D) materials have attracted huge interest being promising candidate for the downscaling of technological devices. Exfoliation techniques to get thin specimens have boosted the research in this field. Among these materials, CrCl3 is facing a renewed attention exhibiting weak van der Waals interaction between the layers as well as in-plane ferromagnetic order[1]. We have exfoliated few layers of CrCl3 flakes from its bulk counterpart on the precleaned Si substrate with 270nm thermally oxidized dielectric SiO_2 layer.



We used to store the material under the glove box to avoid the oxidation because chromium trihalides are very prone to oxygen and atmospheric humidity. Flakes of $CrCl_3$ were transferred on the substrate through mechanical exfoliation by using scotch tape. After transferring the flakes on the substrates, we preferred to clean the samples under three subsequent baths on the hot plate at 40°C for 10 minutes in aforementioned liquids. By following this process, we remove the glue between the substrate and layers.To identify the transferred layers, we followed the previous mentioned reliable techniques[2] i.e. optical microscope, atomic force microscopy and Raman spectroscopy. Figure 1(a) shows the optical image of $CrCl_3$ thin flake, which attain the optical contrast $\backsim$0.026. In Figure 1(b), we showed the AFM image of same flake. By the analysis, we found that the thickness of the layer varies from 80-100 nm. Here, we confirmed the few layers of $CrCl_3$ with optical analysis.

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Optical readout of radio-frequency signals with a multimode opto-electro-mechanical transducer

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An opto-electro-mechanical system formed by a nano-membrane capacitively coupled to an LC resonator and to an optical interferometer has recently been proposed and employed for the highly sensitive optical readout of radio-frequency signals. We propose and experimentally demonstrate how the bandwidth of such a transducer can be increased by controlling the interference between two electromechanical interaction pathways of a two-mode mechanical system. We have realized a device based on a SiN nanomembrane coated with a 30 nm-thick Nb film which is coupled to an LC resonator and optically readout by an interferometer. Operating this proof-of-principle device at room temperature, we achieve a sensitivity of 300 nV/Hz over a bandwidth of 15 kHz in the presence of radio-frequency noise, and an optimal shot-noise-limited sensitivity of 10 nV/Hz over a bandwidth of 5 kHz.

We discuss strategies for improving the performance of the device, showing that, for the same given sensitivity, a mechanical multimode transducer can achieve a bandwidth significantly larger than that for a single-mode one by creating constructive interference between the two opto-electro-mechanical interaction pathways. The nature of the interference can be controlled by choosing proper electrode configurations with respect to the membrane vibrational modes involved and we also show that such an interference allows to create nonreciprocal transmission between optical and radio-frequency signals.

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Car-Parrinello Molecular Dynamics Simulations of High Temperature GeO2

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Thanks to its higher electron and hole mobilities and its lower operating voltages, germanium is gaining increasing consideration for replacing silicon for less energydemanding solid state devices. A series of first-principles molecular dynamics simulations have been carried out for a relatively large system consisting of 240 GeO2 atoms. We have covered the entire range 10-4000K by *ab-initio* simulations using norm conserving, separable, dual-space gaussian pseudopotentials for the BLYP exchange-correlation functional. The high temperature results show structural properties which are in good agreement with experimental results encouraging for further simulations at lower temperatures to get a representative GeO2 system.

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Structure of melts under high pressure and high temperature conditions by X-ray absorption spectroscopy

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Nowadays X-ray Absorption Spectroscopy (XAS) is a powerful and established tool to investigate solid and liquid matter at high pressure and high temperature (HP-HT). Such experiments rely on the high pressure technology whose continuous development has extended the achievable range up to the multi Mbar regime. In such devices, the high temperature conditions needed to access the molten state are typically obtained by using internal resistive heaters or by laser heating the sample. We have recently developed an internally heated diamond anvil cell (DAC) allowing measurements up to 1100 K (or even more) with the capability to performed heating and cooling ramps faster or comparable to what can be done with large volume cells or external heating in DAC. Such fast heating/cooling rates are suitable for studying melting/crystallization dynamics when coupled with an energy dispersive XAS setup. Within this contribution, we describe this internally heated DAC device which has been realized and tested in experiments on molten Selenium (Se) performed at the energy dispersive ODE beamline of Synchrotron SOLEIL. We also present some results obtained from the experiments carried out on elemental Se using a large volume Paris-Edinburgh press.

Assessment of problem solving activity on waves and modern physics in secondary school

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Students of Italian secondary school have difficulty dealing with the study of waves and modern physics. These are two interrelated subjects because of the wave-particle duality of quantum systems. Hence, a sound knowledge of wave phenomena is a mandatory prerequisite for learning quantum mechanics. We developed conceptual problems on these topics and tested them in a design-based research framework1, in order to understand:

I What naïve conceptions do students hold related to this subject matter?

II Is the discussion of conceptual problems effective in improving learning outcomes?

We proposed the activity on waves to fourth-year students (278 students for Module 1 and 261 for Module 2) and the activity on modern physics to fifth-year students (139 students for Module 3 and 77 for Module 4). All students had previously received formal instruction on these topics. Students worked out the problems in groups, then they were involved in a guided classroom discussion. To assess the effectiveness of our intervention, we developed a multiple-choice questionnaire, which was administered as pre- and post-test. We performed a classical item and distractor analysis and calculated the effect size via Cohen's d. Our findings so far confirm what is known from research literature on the common naïve conceptions on these topics, like the idea that the frequency affects the propagation speed of a wave in a homogeneous medium2 and that every spectral line is associated to an atomic energy level3. Our analysis also reveals that the discussion of conceptual problems can be effective in improving student understanding (the effect size is 1.8 for Module 1, 0.9 for Module 2, 1.0 for Module 3, 2.4 for Module 4). In the future, we plan to focus on a smaller sample, recording interviews and field observations, and analyzing them qualitatively, to investigate how students' ideas evolve during the activity.

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Spectroscopic signatures of coated nanoparticles modification in LMO cathodes for Li+ batteries

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The lifetime and safety of batteries must be priority matter of investigation, if possible, even more than capacity itself. Use of LMO (Lithium Manganese Oxides) as a reasonable substitute of LCO in positive electrodes make us extremely confident about the future improvement of safety in all the applications. In these classes of systems, transformation from the spinel to the layered structure requires Mn migration from one octahedral site to another, through an intermediate tetrahedral site. This process has a high energy barrier and will not likely take place unless it is aided, for example, by charge disproportionation in the tetrahedral site. Such circumstances are unlikely in the bulk of the sample, in which most of the Mn ions are in the 4+ oxidation state, therefore explaining why the spinel structure retains its phase in the bulk. However, previous XPS analyses, indicated that near the particle surfaces the valence of Mn is lowered to Mn3+ and Mn2+, enabling the requisite charge disproportionation process and making manganese migration possible. [1] From these signatures we intend to depict the landscape of possible future advancements like high lithium transfer in LMO (more than 50than in Co could promote Mn among the safest electrodes. Under standard battery operation conditions, we have applied in-situ soft X-ray Absorption Spectroscopy (XAS) revealing enhanced Mn(II) content at LMO/liquid electrolyte interfaces during battery charging, and reduced Mn(II) surface concentration during discharge [2] when working at low voltage . This is paradoxical, as more Mn(IV) are expected during the charging process. In the present work we use of an alumina coating to reduce Mn(II) from an amount of almost 100In particular we focus on the morphological implications occuring in the charge/discharge process. In particular during the Li ions intercalation in the cathode at 3V through the 8a-16c- 8a-16c path produces a fast diffusion of Li that will bring to a first order transition to a cubic structure and consequent volume expansion. In this study we observed by SEM a straightforward modification of the morphology due to the opening of Li+ channel at discharge. Organization of morphology is as following: cluster of nanoparticles 20-40 nm are organized to globular structures of diameter > 150 nm while individual nanoparticles which are outside the globular structures are also seen but slightly sparse.

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The sandwich in the middle: two-membrane cavity optomechanics

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Multi-element systems of micro/nano-mechanical resonators offer promising prospects for enhanced optomechanical performances, coherent control, and for the exploration of multi-oscillators synchronization. The standard path for reaching the strong single-photon optomechanical coupling regime is to consider co-localized optical and vibrational modes with a large spatial overlap confined in very small volumes, corresponding to mechanical modes with extremely small effective mass. An alternative solution, capable of providing systems with orders of magnitude increased ratio between the single-photon optomechanical coupling rate, and the cavity decay rate, is to exploit quantum interference in multi-element optomechanical setups. Although the simplest two-membrane sandwich in an optical cavity is a paradigm for the realization of strong-coupling optomechanics, and the observation of collective mechanical effects (such as synchronization), no experimental studies of these phenomena have been reported till now. Previous related results were confined only to the optical and mechanical characterization of two-membrane sandwiches. Here we report on the first experimental characterization of the optical, mechanical, and especially optomechanical properties of a sandwich constituted of two parallel membranes within an optical cavity. We show how the resonance frequencies of the optical cavity are shifted as a function of the position of the two membranes. This effect is central to the description of the optomechanical properties of the system, since it provides a direct estimation of the strength of the couplings. By investigating the shifts of the cavity resonances, we find that the optomechanical coupling strength is enhanced by constructive interference when the two membranes are positioned to form an inner cavity which is resonant with the driving field. Specifically, we determine a gain of $\backsim 2.47$ in the coupling strength of the relative mechanical motion with respect to thesingle membrane configuration. We finally prove both the capability to tune on demand the single-photon optomechanical couplings, and the simultaneous optical cooling of the fundamental modes of the two distinct membranes.

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Machine learning for quantum matter

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Machine learning techniques are at the core of various everyday life technologies, like speech recognition software, on-line recommender systems (e.g., youtube and Netflix), and autonomously driving cars. They have already proven to be useful tools also for condensed-matter and quantum-chemistry research. Here, they have been employed to solve hard computational tasks, such as determining force fields for molecular dynamic simulations1, predicting protein-ligand affinities in computational drug design2, or computing atomization energies of crystals and molecules3. In this work, we explore the use of supervised machine learning to predict properties (such as energy levels or dynamical response functions) of complex quantum manybody system. The main focus is on experiments performed with ultracold atomic gases trapped in disordered external fields created using optical speckle patterns. Specifically, a deep neural network is trained to reproduce the low-lying energy levels of a quantum particle in the speckle field, using as a training set a large number of instances of the speckle field whose energy levels have been preventively determined via a high-order finite difference technique. Remarkably, we find that a neural network with a sufficient number of hidden layers can accurately predict the energy levels of previously unseen instances of the speckle field. This finding paves the way to new strategies to speed up computationally expensive quantum mechanical calculations for ab-initio atomistic simulations and for computational docking in drug design research.

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Comparative study of many-body t-matrix theories for a Fermi gas through the BCS-BEC crossover

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In the latest several years, diagrammatic theories based on the t matrix approximation with different degrees of self-consistency have been developed to describe a Fermi gas through the BCS-BEC crossover [1,2,3,4]. A comprehensive comparison between the results obtained by the different approaches for both thermodynamical and dynamical quantities is, however, still lacking. In the present work, we consider all the possible ways of implementing self-consistency in the t matrix approximation and we compare the outcomes of the different approaches between each other (and with the available experimental and Quantum Monte Carlo data) through the whole BCS-BEC crossover. In this way, we expect to provide a guideline on the virtues and the drawbacks of each scheme that can help future research in this field.

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Modeling and simulations of carbon pseudospheres

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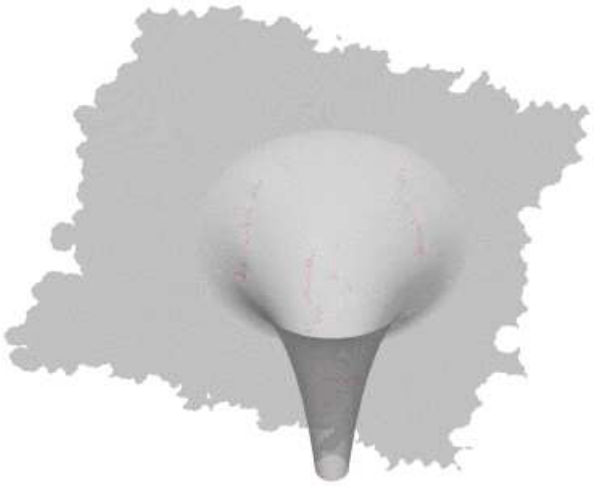
In a previous work it was shown that the realization of the graphene topology on a Beltrami pseudosphere may lead to experimenting the analogue of the Hawking-Unruh effect on a condensed matter system [1]. This effect predicts that quantum fields in curved space-time with an horizon exhibit a thermal character due to the quantum vacuum and to the relativistic process of measurement. The aim of this work is thus to produce a 3-coordinated carbon structure on a Beltrami pseudosphere to find the minimal energy configuration of the atoms on this surface, showing that it is energetically stable and, thus, that can be obtained experimentally. Heptagonal and pentagonal defects (represented in blue in the figure below) emerge on the surface due to the negative curvature [2]. We devise a new algorithm to scale-up the pseudospehere dimensions reaching a radius of the event horizon (maximum circumference) R 200 nm. Next, we study the curvature effects on the electronic properties of the system, which should bring about a thermal spectrum in the form of finite temperature electronic Local Density of States [1].



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Probing the lithium storage mechanism in transition metal doped ZnO anodes by x-ray absorption spectroscopy and diffraction

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Li-ion batteries (LIB) are the state-of-the-art power sources for portable electronics. Nonetheless future large scale applications such as, for instance, electric vehicles require novel cathode and anode materials with enhanced energy and power density along with long term cycling stability. For the anode site, a new class of materials, combining the conversion and alloying reaction mechanisms in one single active compound has gathered continuously increasing interest. Within these materials, transition-metal-doped zinc oxide has been reported as a very promising alternative anode material for Li-ion batteries[1]. The introduction of Fe or Co into the wurtzite structure results into an enhanced reversible capacity exceeding 900 mAh/g (almost three times higher than in pure ZnO) and improved cycling stability even at high rate. The further optimization of such class of materials requires the understanding of the electrochemical (de-)lithiation reaction mechanism at the atomic scale.

Within this contribution, we report the results of our recent XAS and XRD investigations of $Zn_{1-x}Fe_xO$ and $Zn_{1-x}Co_xO$. Samples were prepared through sucrose assisted wet chemical synthesis. Crystalline structure and average crystallite size were determined by refinement of the XRD patterns measured for different dopant species and concentrations. Synchrotron radiation X-ray absorption spectroscopy (XAS) has been used to probe oxidation state and local structural environment of the transition metals both on the pristine material[2,3] and on anodes measured ex-situ and in operando during galvanostatic cycling[4]. The present study provides a full characterization of the different crystalline but also amorphous and nanocrystalline phases that commonly form upon Li-uptake/release and fundamental insight into the mechanism of the conversion/alloying reaction in this class of materials.

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XAS and Reverse Monte Carlo studies of structure and atomic correlations in molecular systems and liquid metal alloys

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X-ray absorption spectroscopy (XAS) has the capability to provide precise atom specific information on the average distribution of the nearest neighbours, and beyond the pair correlations when combined with suitable data analysis strategies. In our previous studies, Reverse Monte Carlo (RMC) modelling of XAS data[1] has been applied to provide a complete insight into the atomic correlations at the microscopic level and address important issues, such as the presence and extent of local icosahedral ordering in liquid close-packed metals[2,3].

Within this contribution, we report our recent developments of the RMC-GNXAS method[4] and newly added features including multi-atomic and multiple-edge refinements. A few applications of RMC to XAS and diffraction data of several gas-phase molecules and binary alloys will be presented.

RMC-GNXAS has been used for the analysis of x-ray absorption spectroscopy (XAS) multiple-edge data sets for six gas phase molecular systems (SnI_2, CdI_2, BBr_3, GaI_3, $GeBr_4$, GeI_4)[5]. Sets of thousands of molecular replicas were involved in the simultaneous refinement of XAS data and electron diffraction results. The validation of this approach on simple molecular systems is particularly relevant as a basis for the method application to more complex and extended systems including metal-organic complexes, biomolecules, or nanocrystalline systems.

For liquid Sn-based metallic binary alloys[6], the combination of XAS and RMC allowed us to obtain three-dimensional models of the local structure compatible with present experimental evidence overcoming some limitations of standard approaches.

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Cavity optomechanics with feedback-controlled in-loop light

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Feedback loops based on real-time continuous measurements are commonly used for stabilization of classical and quantum systems. Typically a system is continuously monitored via a probe electromagnetic field, and the acquired signal drives the actuator which in turn drives the system to the desired target. Here we demonstrate a novel closed-loop control scheme in which the actuator acts on the probe field itself in order to engineer its phase and amplitude fluctuations. The resulting feedback-controlled in-loop field is then exploited to manipulate the system and improve its performance. In-loop optical fields have already been employed in the negative feedback regime for noise suppression and stabilization, the so-called "squashing". Here, instead, we operate in the "anti-squashing" regime of positive feedback and increased field fluctuations, and demonstrate the potentiality of this new technique by improving the sideband cooling of a nanomechanical membrane by 7.5 dB. In the fully quantum regime, feedback-controlled light would allow going below the quantum back-action cooling limit. We also show that a weakly coupled optomechanical system at room temperature can manifest normal-mode splitting when the pump field fluctuations are antisquashed by a phase-sensitive feedback loop operating close to its instability threshold. Under these conditions the optical cavity exhibits an effectively reduced decay rate, so that the system is promoted to the strong coupling regime. In this regime one can observe coherent energy exchange and optomechanical oscillations also with a weakly coupled system, Finally, we describe how the feedback that operates by measuring the light leaking through a cavity output may be properly engineered to enhance the ponderomotive squeezing of the light leaking through another cavity output.

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