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5^{th} Scientific Day of School of Science and Technology, UNICAM

Book of Abstracts

Camerino
June 8, 2016

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Camerino, 8 June 2016

Dear Colleagues,

this year the Scientific Day of the School of Science and Technology (SST) is at its fifth edition. As for the past editions, the young researchers of our School are the main protagonists of this event through the presentation and discussion of their scientific achievements. The Scientific Day thus represents a showcase of various topics that are presently ongoing in our research groups. The target of this meeting is to stimulate discussion among researchers and foster interdisciplinary collaboration toward the start up of common research projects.

Since the last edition of the Scientific Day held in 2014, an increasing number of grants and doctoral positions obtained by our scientists are the result of contracts and agreements with private enterprises. This is a valuable achievement that very often generates a strong connection between academia and the companies which are active part of the productive development of our territory. Excellence in research is also nurtured by basic research, mainly funded by public agencies, especially at European level. A special effort is thus required in order to boost the growth of new ideas that would bring to successful applications to the European Commission grants.

This is a really demanding task that I hope, within its limits, this Scientific Day will contribute to reach.

The Dean of the SST
Marino Petrini

Contents

Chemistry

Developing a new method to analyse volatile substances in extra virgin olive oil

Aurini G.[1], *Concettoni E.*[1], *Lanero F.*[1], *Panni F.*[1], *Galiè V.*[1], *Boarelli M.C.*[1], *Fiorini D.*[1]

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The applications of gas chromatography in the field of food science are of great importance for the assessment of food quality and safety. As an example, volatile compounds are key molecules in the definition of the overall quality of extra virgin olive oil[1]. New methods to analyse volatile substances in olive oil by solid-phase microextraction and gas chromatography coupled to mass spectrometry are currently under investigation in our laboratory. Interesting preliminary results show that the aqueous extract of olive oil can provide the same result as when the analysis is carried out on the oil as such, with the advantage that the oil aqueous extract is much easier to handle, the solid-phase microextraction fiber assembly used has a much longer lifetime and the use of an internal standard is allowed, while using the oil as such, the homogenization of the internal standard is practically unfeasible. The results of the study will be presented and discussed.

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Nematic director configuration, local order and microviscosity in a PSLC cell

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The director configuration, the local order and the molecular-level reorientational dynamics (microviscosity) of the 5CB liquid crystal (LC) inside a polymer-stabilized LC (PSLC) cell prepared with the 4,4'-bis(6-(acryloyloxy)hexyloxy)biphenyl (BAB6) diacrylic monomer have been studied with the EPR spin probe technique [1], already used for other liquid crystal devices [2,3], across the nematic and the isotropic phase of the LC. The cells made from glass slides, either clean or coated with an aligning layer, were filled with pure 5CB or with 0.5, 1.0 or 2.0 wt % of BAB6, either in the monomeric state or polymerized. Local orientational order parameter (<P2>) in the non treated cells was always slightly lower than in the coated ones and both were lower than in the bulk LC. Order appeared to be independent of polymerization state or BAB6 concentration up to 1.0 wt %. Reorientational dynamics was essentially bulk-like in all cases, indicating that in our PSLC cells a full molecular mobility is retained. At the concentration of 2.0 wt %, in the coated cell with polymerized BAB6, the monodomain did not reform after a 90° rotation of the cell in the magnetic field, suggesting that the polymer network is, as expected, stabilizing the preexisting director configuration.

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Antioxidant Natural Compounds from African Medicinal Plants

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Twelve compounds were isolated by antioxidant-guided phytochemical investigation of the MeOH extracts of *Cordyline fruticose* and *Eriobotrya japonica*[1]. The compounds were identified as: Farrerol, quercetin helichrysoside, apigenin 8-C-β-D-glucopyranoside, isoquercitrin and rutin (*C. fruticose*), β-sitosterol, catechin, oleanolic acid, lyoniresinol, cinchonain IIb, lyoniresinol 2-a-O-β-D-xylopyranoside and β-sitosterol-3-O-β-D-glucopyranoside (*E. japonica*). Helichrysoside and rutin from *C. fruticosa*, and catechin, cinchonain IIb and lyoniresinol 2-a-O-β-D-xylopyranoside from *E. japonica*, showed interesting antioxidant activity, with EC50 of 8.73, 9.91, 4.11, 3.14 and 10.61 μg/mL, respectively.

A new C-glycosylflavone, drymaritin E (6-C-(3-keto-β-digitoxopyranosyl)-4'-O-(β-D-glucopyranosyl)- 7-methoxyl-5,4'-dihydroxylflavone) 1 was isolated from the MeOH extract of the aerial parts of *Drymaria cordata*[2]. Two known compounds (cassiaoccidentalin A 2 and anemonin 3) and an inseparable mixture of two known C-glycosylflavones 5,4'-dihydroxy-7-methoxyflavone-6-C-(2"-O-α-L-rhamnopyranosyl)-β-D-glucopyranoside 4a and 5,7,3',4'-tetrahydroxyflavone-6-C-(2"-O-α-L-rhamnopyranosyl)-β-D-glucopyranoside 4b were also isolated. The alkaline hydrolysis of 3 led to a new hemisynthetic derivative, sodium anemonate 3a. The C-glycosylflavones showed significant free radical-scavenging activities on the radical 2,2-diphenyl-1-picrylhydrazyl (DPPH). In particular, compound 1 exhibited a concentration-dependent radical scavenging activity on DPPH with EC50 of 31.43 μg/mL.

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A system to analyse volatile organic compounds emitted during cooking

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There is nowadays more awareness on the impact on health of pollutants emitted even during cooking both from commercial as well as from domestic activities. Cooking processes like frying, roasting, grilling, boiling and broiling, contribute to emissions of pollutants, particularly in closed, poorly ventilated areas where air quality is deeply influenced on their presence[1]. Volatile organic compounds (VOCs) are a large group of carbon-based chemicals that easily evaporate at room temperature, but while some VOCs are odorous, many of them can not be detected by our senses, even if their inhalation may be associated with health risks[2]. Thus, given the importance of monitoring VOCs emissions during cooking activities, the objective of this study is to set up and assess the applicability of a new system allowing to analyse these compounds. In order to address this task, air samples obtained from different cooking techniques, were sampled in olfactometric bags and analyzed using solid-phase microextraction and gas chromatography coupled to mass spectrometry (SPME-GC-MS). The bag allows to transport the sample to the instrument location and to perform the SPME extraction of the sampled air. Despite several applications have been developed in different field, this kind of sampling system combined to SPME-GC-MS, has never been exploited to study the emissions of VOCs formed during cooking and based on the first results, it seems to be successful to this purpose. Thus, preliminary results will be presented and discussed.

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Charge transfer complexes with coinage metals trinuclear metallocycles (CTCs) and TTF, DBTTF and BEDTTF.

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Charge-transfer complexes are combinations of charge-donor (D) and charge-acceptor (A) materials. While the parent compounds can be unipolar semiconductors, the CT complex can have entirely different properties; it can be an ambipolar semiconductor, a metal conductor at the interface, or even a superconductor.[1] In the last years a comprehensive study on coinage metals coordination chemistry has established new perspectives on the application of CycloTrimer Compounds (CTCs).[2] From elegant examples of the coordinative skills of 11th group metals, they have been promoted as building blocks for materials with sophisticated features in the field of luminescence, optoelectronics and as photovoltaic materials. This promotion is mainly due to the fact that the CTCs showed to possess ?-acid or ?-basic characters on the regards of metal cations, organometallic frameworks or organic molecules according to the nature of the central metal, of the azolate bridging ligand or of the substituents on it.[3] By mixing solutions of the corresponding Cu(I), Ag(I) and Au(I) CTCs and different donor organic compounds such as TTF (TetraThioFulvalene), DBTTF (DiBenzoTetraThioFulvalene) and the BED-TTF (Bis(EthyleneDithiolo)-TetraThiaFulvalene), 12 new CT derivatives with a mole ratio A/D of 1 : 1 or 1 : 2 have been isolated as stable solids and characterized both in solution (^{1}H NMR and UV-visible spectroscopies) and in the solid states. Six of them have also been characterized by preliminary X-ray diffraction structural determinations showing the stacking assemblies and the local structural distortions due to the strong interactions.

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Sol-Gel Synthesis of Iron-Manganese Mixed Oxide as Superior and Eco-Friendly Anode for Lithium-Ion Batteries

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Lithium-ion batteries (LIBs) are the perfect balance between portability, low cost and good performances. Considering the anodic side, graphite is the most used active material[1], which despite its wide use, and a specific capacity of 372 $mAhg^{-1}$, has been included in the European Commission list of critical raw materials that have to be replaced in the future. For this reason, a great deal of effort has been devoted to investigate a relatively new class of materials emerged in this last few years, showing a different reactivity from traditional insertion materials, the so-called conversion materials. Among these, transition metal oxides (TMOs), can reach extremely high capacity values, up to five times higher than graphite[2]. Despite this, they have evidenced several drawbacks: short cyclic life, a large first cycle irreversible capacity, and a relevant volume variation during cycling. In this work, an Iron-Manganese mixed oxide was synthesized by Sol-Gel method and tested as anode for Li-ion batteries. In order to address the aforementioned drawbacks, and improve the mechanical stability of the electrodes, improved binders with superior mechanical properties[3], such as Polyacrylic Acid (PAA) and Sodium-Carboxymethyl Cellulose (Na-CMC), and an environmentally friendly electrode processing using ethanol or H2O as solvents, were evaluated. The experimental data shown superior performance with respect to the standard Polyvinylidene Fluoride system, which makes use of the expensive and toxic N-Methyl-2-pyrrolidone (NMP) solvent.

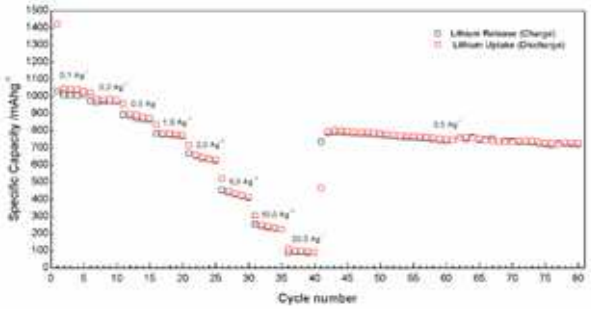

Figure 1. Iron-Manganese mixed oxide performance at different current density.

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$CeCl_3 \cdot 7H_2O$/NaI as Lewis acid catalyst in the Povarov reaction for the synthesis of functionalized tetrahydroquinolines

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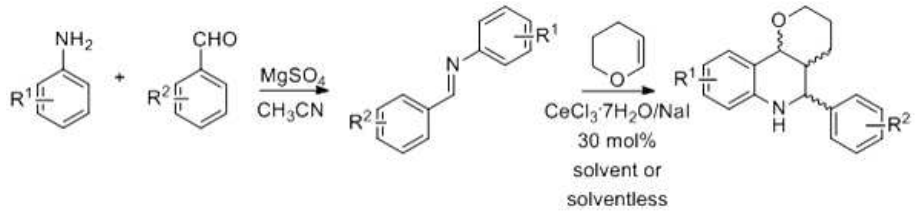
Many different biologically active compounds contain the widespread scaffold of tetrahydroquinolines[1]. Hence the interest toward their synthesis has stimulated the development of several synthetic strategies, among which the Povarov reaction is one of the most applied. The performance of this three-components imino Diels-Alder reaction can be improved by Lewis acid catalysis. In the last years the search for more economic and environmentally benign synthetic methodologies has stimulated the use of nontoxic and nonexpensive catalytic systems, and in this perspective Cerium trichloride has became interesting because of its low toxicity and cost and for the ease of application also in non anhydrous conditions.[2,3] Here we describe the study of the $CeCl_3 \cdot 7H_2O$/NaI system as Lewis acid catalyst in the Povarov reaction for the synthesis of substituted tetrahydroquinolines.



Scheme 1 - Synthesis of terahydroquinolines through $CeCl_3 \cdot 7H_2O$/NaI catalyzed Povarov reaction.

The reaction proceeds well, in acceptable reaction times and up to 86% yield. Both syn and anti diastereomers of the final tetrahydroquinoline can be obtained preferentially, depending on the reaction conditions, because the stereoselectivity is opposite in acetonitrile or in solventless conditions. Also substituted anilines and aromatic aldehydes have been employed with good results. A further investigation was made about the mechanism, to understand the formation of the main byproducts.

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Development of Antibacterial Carbon Filters for Air Treatments

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Alternative materials for indoor air treatment were developed by combining the well-known porosity of carbon materials1[1] and the antibacterial activity of ruthenium-curcuminato complexes.[2] Different types of carbon were used to study the influence of their physicochemical properties and ruthenium complexes were selected based on their solubility and toxicity.[3] The stability of complex on carbon surfaces at low loading (1% wt) and their antibacterial activity was analyzed by different techniques. The combination of low soluble Ru-complex with high porous carbon materials guarantees the avoidance of leaching even in solution and leads to materials with remained high porosity and adsorption capacity in addition to antibacterial activity. All materials remain free of bacteria even after three days in a high concentrated bacteria cultivation media.

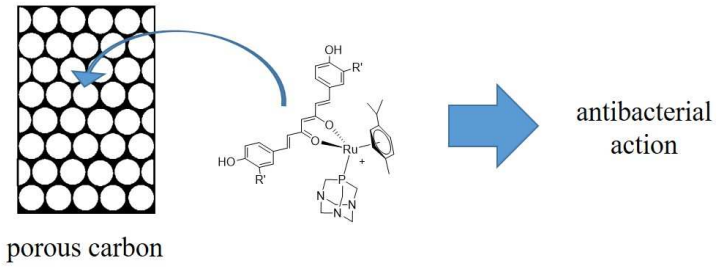

Figure 1

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The global energy demand: photocatalytic systems for hydrogen production.

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The continuous economic growth due to the world's expanding population results in an increase of global energy demand. The world energy consumption mainly concerns the use of fossil fuels followed by hydro and nuclear energy; the remaining part belongs to the renewable energies sources. The develop of alternatives for the generation of sustainable energy is an important research field which attracts much attention, since the fossil fuels are an energy sources that will exhaust in the coming decades[1]. An important process is the conversion of solar energy into chemical ones[2] as happens in the natural photosynthetic process. Different research focused their works on the optimization of artificial system that reflects the photosynthesis in which the aim is to harmless the sunlight energy in combination with a catalytic system to conduct the photocatalytic water splitting in order to form oxygen and hydrogen[3]. The research work developed in the Professor S. Rau's research group, at University of Ulm, focused on photocatalysis targeted to the production of hydrogen using different photocatalysts in two different assembly: intramolecular and intermolecular systems. The study was divided in two parts, the aim of the first one is to find a new synthetic pathway, in order to obtain a pure intramolecular photocatalyst $[(tbbpy)_2Ru(tpphz)PtI_2](PF_6)_2$ for the photocatalytic hydrogen production. This photocatalyst was already synthetized in a not pure form in Rau's research group by Dr. Pfeffer[4]. The second parts compared the functioning in term of hydrogen catalytic efficiency of two intermolecular photocatalysts constituted by different ruthenium complexes as $[(tbbpy)_2Ru(tpphz)](PF_6)_2$ and $[Ru(tbbpy)_3](PF_6)_2$ with the same catalytic centre represented by $[(tbbpy)PtI_2]$ compound.

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Nitroalkanes as Key Starting Materials for Synthesizing 1,2-Diketones

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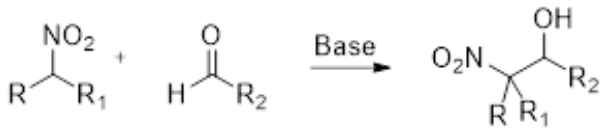
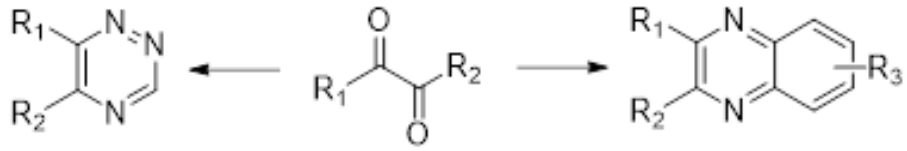
Nitroalkanes constitutes one of the most valuable class of starting materials in organic synthesis[1]. In fact, due to the high electron-withdrawing power of the nitro group, it is possible to generate the corresponding nitronate anion under very mild reaction conditions, and used as nucleophiles with a variety of electrophilic systems[2]. In this context, the Henry reaction is the most important reaction involving nitroalkanes, which consists in a nitroaldol addition between nitroalkanes and aldehydes to afford, under basic reaction conditions, the corresponding ß-nitroalcohols (Scheme 1)[3].



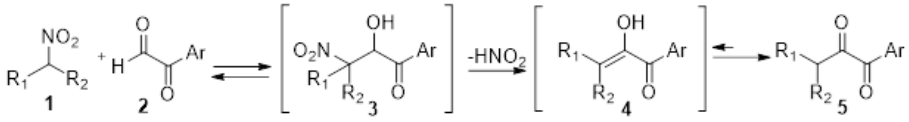
Scheme 1.

Following our studies concerning the chemistry of nitroalkanes, we found a new practical application of the Henry reaction to synthesize 1,2-diketones, which in turn, are valuable intermediates for assembling important heterocyclic systems (Scheme 2)[4].



Scheme 2.

Our approach involves the formation of 3-nitro-2-alkanols 3 that undergoes to the irreversible loss of nitrous acid vs. the conventional water elimination leading to the title targets 5 (Scheme 3).



Scheme 3.

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Analysis of Rubber Samples for Forensic Purpose

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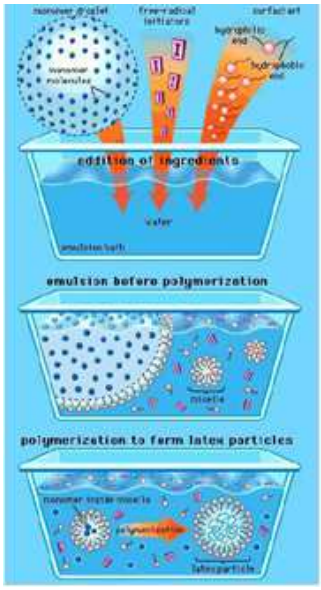
Rubber is commonly encountered material in the human environment in the form of rubber objects such as car tires, shoes (soles), various tool handles and rubber profiles for windows. All these items are not 100% rubber, although rubber is the most important component. The tread of these compounds is that they have numerous ingredients used to make the final product. The choice of ingredients is crucial to help match polymer properties with process and performance needs of their specific applications. The rubber group is the class of ingredient with the least variation, although is present in the greatest amount. The fillers and extender oils are next in abundance, and it is the carbon black filler that gives the tire its black color. All these particles and particle defects in rubber production and post modification, very often can be a valuable source of issues. Chemists became forensic scientist meanwhile all the issues needs to be studied and solved. This is due to the fact that, chemical analysis of rubber is a difficult task because of the specific physicochemical features of rubber, limited transmission of electromagnetic radiation in the IR range, large amounts of additives such as carbon black or silica. Therefore, it is easy to understand that the application of standard analytical methods used in forensic practice in analysis of polymer is very difficult, and the chemist has to look for other methods. In particular, Thermogravimetric analysis (TGA) and Scanning Electron Miscroscopy (SEM) represent very useful methodologies in order to find out the problem related to the cause and possible solutions, in co-operation with the Industry.



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Synthesis of New Climacostol Analogues: a Natural Molecule Become a Lead Compound

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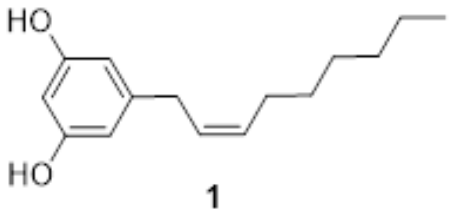
Climacostol[1] is a natural molecule employed by heterotrich ciliate Climacostomum virens as defensive toxin against predators. Climacostol demonstrated to exert a cytotoxic effect on a panel of human cell lines with activation of either apoptotic or apoptotic-like cell death, and negligible effect on non-tumor cells[1,2]



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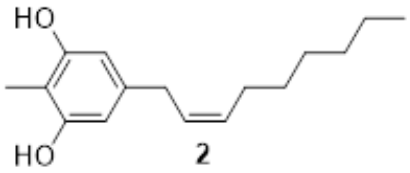
In this study, we synthesized two derivatives of climacostol with different substituents on phenyl ring. The strategy for these molecules include a crucial Wittig reaction that allows to obtain just the (Z)-isomer and not the inactive form (E)-isomer[3]. In addition to the future work of synthesis, the study continues in research in vivo tests to study the biochemical activity of our derivatives.



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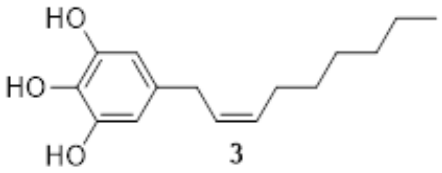

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Study of the Pyrolysis of PMMA to Improve its Recyclability

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The worldwide rapid industrialization and population growth have exponentially increased the production and consumption of plastics in various fields (Figure 1), which has created serious social and environmental arguments in the disposal of wastes. In this regard, recycling of plastic wastes could be an interesting alternative in the environmental and energy saving/waste management point of view. Contaminated plastic wastes can only be partly recycled into new products while some plastics can completely be recycled into its original monomeric form by depolymerization, such as, poly(methyl methacrylate) (PMMA)[1]. PMMA is a major type of thermoplastic used throughout the world in such applications as transparent all-weather sheets, electrical insulation, bathroom units, automotive parts, surface coating, ion exchange resins, etc[2]. Thermal degradation of PMMA is a quantitative chemical reaction in which the polymer chains are decomposed to its monomeric form at high temperature[3]. We studied thermal degradation of PMMA by pyrolysis using thermogravimetry coupled with mass spectrometry (TGA-MS) and found that the major product of degradation was MMA, besides traces of methyl pyruvate and 2,3-butanedione along with the main by-product methyl isobutyrate. The generated by-products were responsible for unpleasant smell in recycled MMA/PMMA as well as for reduced property of recycled PMMA. Thus, elimination of the by-products was essential for the production of a material which can be used in safer industrial and consumer products.

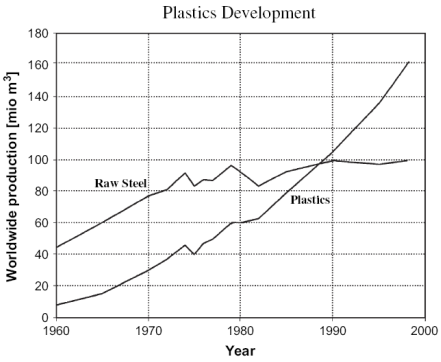

Fig. 1. Plastics production compared to steel production.

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Quaternary Ammonium Salts as Highly Efficient Biocides in the Treatment of Microbial Degradation of Artworks

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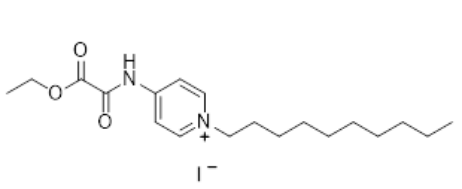
Quaternary ammonium compounds (also known as quats or QACs) have been widely used as antimicrobials and disinfectants in the last decade[1], mainly due to their enhanced property to induce morphological changes and cell autolysis[2] in both gram-positive and gram-negative bacteria, combined with their extremely low toxicity for human cells. In order to have the hydrophobic behaviour required to fulfill the biocidal activity, it has been established that the alkyl substituent chain on the quaternary nitrogen atom should consist in a chain of 8-18 carbon atoms[3]. Moreover, the positive charge on the nitrogen atom seems to play a key role in the mechanism of these compounds, since they are attracted by the negatively charged phosphate groups in the cellular membrane of the microbial cells. This study describes the synthesis and characterization of two QACs, the 1-decyl-4-(2-ethoxy-2-oxoacetamido)pyridin-1-ium iodide (1) and the (S)-N-(1-ethoxy-3-hydroxy-1-oxopropan-2-yl)-N,N-dimethyldodecan-1-aminium iodide (2).



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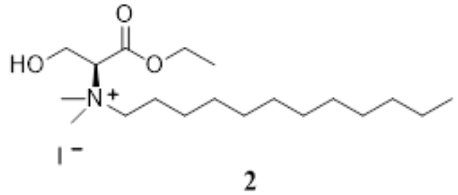

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These two compounds have shown a remarkable activity against the proliferation of micro-organisms responsible for the degradation of numerous artworks, such as fungi that easily colonize the surface of monuments, or bacteria responsible for the loss of colour in paintings.

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Ecofriendly flame retardant fillers: natural magnesium hydroxide and aluminium hydroxide produced by milling.

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Unwanted fires account for significant losses to life and property and organic polymers fuel their vast majority. Since the flammability of a material is not an intrinsic property, changing the material composition, for example by the addition of a fire retardant, will also change its reaction to fire behavior, hence reducing fire losses, fire injuries, and deaths. A wide variety of flame-retardant additive compounds is in use, enabling materials with an otherwise poor fire performance to fulfill regulatory fire performance criteria.[1]. Flame retardancy of polymers is often achieved by the addition of compounds containing elements such as halogens, nitrogen, or phosphorus, but the combustion products are toxic compounds such as acid gases, HCN, and environmental toxins. For this reason, in the last decades, the research of the scientific community is focused on the development of "greener" flame retardant systems able to minimize toxic products and environmental hazards by using selected metal hydroxide[2−5]. Their fire retardancy is primarily a result of a strongly endothermic decomposition with the release of water, and they do not introduce any corrosive or potentially toxic substances. Aluminum and magnesium hydroxides (ATH and MDH) are the most effective products. In this regard, Nuova Sima srl was a pioneer in the production of natural MDH (Hydrofy) by milling the mineral Brucite[6]. Nuova Sima srl produces also ATH (Alufy) by milling an intermediate product of the Bayer process. Nuova Sima products list comprises a great variety of materials with different particle size and their research activity is centered on the development of new surface modification both to improve the compatibility between such mineral fillers and polymers and to optimize the effect on mechanical and electrical properties.

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The "golden era" of carbenes: chemistry of coinage metals N-Heterocyclic Carbene complexes as anticancer drugs

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The fascinating chemical properties of N-heterocyclic carbene (NHC) complexes showed them to be a suitable class of complexes to be investigated for their applications as drugs in the treatment of the infectious disease or cancer. In particular, the great structural versatility provided a library of compounds with a low cytotoxic profile, suitable candidates as new anticancer agents[1]. Their key features are the easy design of the ligand structure that allows the modulation of the hydro-/lipo-philicity balance, responsible for the selectivity against the target tissue.

In the last years, we have developed several classes of coinage metal-NHC complexes obtained from the precursors $\{[HB(HIm^{R})_3]Br_2\}$ (R = Bz, Mes and *t*-Bu), $\{[H_2B(HBzTz)_2]Br\}$, $\{H_2C(HTz^{R})_2\}$ and $H_2C(HImR)2$ (R = $(CH_2)_3SO_3^-$ or $(CH_2)_2COO^-$)[2].

Recently we have focused the research work on new 11th group metal-NHCs complexes obtained from the water soluble ligands $HIm^{1R,3R}Cl$ (R = $COOCH_3$, $COOCH_2CH_3$ or $CON(CH_2CH_3)_2$)[3], the zwitterionic water soluble precursors $NaHIm^{1R,3R}$ (R = $(CH_2)_3SO_{3^-}$)[4], $NaHIm^{1R,3R,4R''}$ (R = $(CH_2)_3SO_{3^-}$, R" = H, CH_3)[5] $NaHBzIm^{1R,3R}$ (R = $(CH_2)_3SO_{3^-}$)[5], $NaHIm^{1R,3R',4R''}$ (R = $(CH_2)_3SO_{3^-}$, R' = Bz, R" = H)[5] and $\{[HBzIm^{1R,3R'}]Br\}$ (R = $(CH_2)_3SO_3Na$, R' = Bz)[5].

More recently we have synthesized and investigated the cytotoxic activity of the novel NHC ligand precursor $[HTz^{(\rho NO_2Bz))_2}]Br$, and the corresponding metal complexes $M[Tz^{(\rho NO_2Bz))_2}]Br$ (M = Cu(I), Ag(I) or Au(I))[6]. We have also carried out a detailed analysis of molecular and cellular pharmacology, allowing to elucidate the role of the metallic core in determining the biological properties.

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Cycling behavior of Magnetite (Fe_3O_4) nanoparticles as anode for Li-ion batteries using PolyAcrylic Acid as improved binder.

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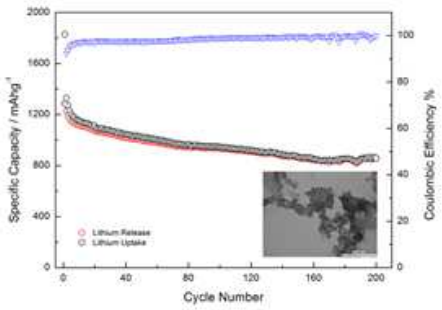
In this last few years, a new chemistry has surfaced with materials able to reversibly store Li by the so-called conversion mechanism[1]: chemical species like transition-metal oxides, phosphides, nitrides have been found to be conversion-enabled species. In this view, Fe_3O_4, also known as magnetite, which is a low cost and environmentally friendly metal oxide, can undertake a reversible conversion reaction with Li+ ions, as shown in equation 1, resulting in a high theoretical specific capacity of 924 $mAhg^{-1}$:

$$Fe_3O_4 + 8e^- + 8Li^+ \rightarrow 3Fe^0 + 4Li_2O \qquad (1)$$

Fe_3O_4 nanoparticles were synthesized by a modified base catalyzed method[2] and tested as anode material for Li-ion batteries. The pristine oxide nanoparticles are characterized by an average size of 11 nm, detected by Transmission Electron Spectroscopy (TEM) imaging. Electrodes were prepared using high-molecular weight Poly(acrylic acid) as improved binder[3] and ethanol as lower cost and environmentally friendly solvent in contrast with the industry-standard Polyvinylidene Fluoride (PVdF) binder, which requires the highly expensive and toxic N-Methyl-2-pyrrolidone (NMP) solvent. Electrochemical experiments showed high specific capacity values of 857 $mAhg^{-1}$ after 200 cycles at a current density of 462 mAg^{-1}.



Fe_3O_4 nanoparticles cycling test - TEM imaging is shown in the figure inset

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Novel coordination frameworks based on N-donor pyrazole derivatives ligands. Characterizations and crystal structures studies

Mosca N.[1], *Pettinari C.*[2], *Marchetti F.*[1], *Pettinari R.*[2], *Galli S.*[3], *Masciocchi N.*[3], *Domasevitch K.V.*[4]

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Metal-Organic Framework (MOFs) or Coordination Polymers (CPs) are crystalline materials consisting in a network formed of single metal ions or metal clusters connected by multidentate organic groups acting as linkers[1]. They generally show strong covalent bonds with high energy, comparable to the single C-C bonds (approximately 350 kJ mol^{-1}). The main MOFs feature is porosity; the theoretical upper limit for MOF surface areas is 14600 m^2/g (one gram of material would cover 2.7 American football fields)[2]. MOFs have found a several range of application[3,4], e.g. in gas storage and separation, magnetism, catalysis, fuel production, water purification, horticulture, drug delivery and heavy metal recovery. Nevertheless, the choice of the metal nodes[5], with a particular attention to their coordination number and to the organic spacers allowed the engineering of MOFs with tuned topologies, pore sizes, and pore-window decorations and then pore functionalization. In this work we report the synthesis, characterization and crystal molecular structures of a series of pyrazolyl-based ligands, namely 3,3'-dimethyl-1H,1'H-4,4'-bipyrazole (H_2Me_2BPz) and 3-nitro-1H,1'H-4,4'-bipyrazole ($H_2BPz^{NO_2}$), (Figure 1) and their MOFs with late transition metals (Co^{2+}, Ni^{2+}, Zn^{2+}, Cu^{2+}, Hg^{2+}, Ag^{+}).

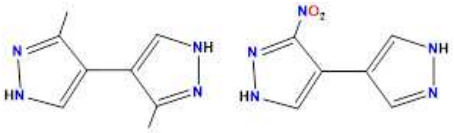

Figure 1

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Investigation of interfacial properties of carbon coated $ZnFe_2O_4$ as new anode material for Li-ion batteries

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In recent years, the growing need for high specific energy density and good cycling performance has prompted the research to develop novel electrode materials for Li-ion batteries. In this context, carbon coated $ZnFe_2O_4$ (C-ZFO) has attracted increasing interest as promising new anode material because it offers an exceptional specific capacity, higher than 1000 mAh g^{-1}, and it is environmentally friendly, non toxic and cheap[1]. This electrode material has been used in SIRBATT project in order to investigate the evolution of Solid Electrolyte Interphase (SEI) in this anode because the performances and durability of batteries are strongly influenced by the passivation layer formed on electrode surface[2]. The electrodes have been prepared by casting the slurry containing active material, conductive carbon and carboxymethyl cellulose as binder. The electrochemical performances and the study of electrode/electrolyte interface have been investigated by galvanostatic cycles at different C-rate values, Electrochemical Impedance Spectroscopy (EIS) at 25°C and 50°C and soft X-ray adsorption spectroscopy (XAS) using synchrotron radiation. The electrochemical results have shown that C-ZFO has good cycling performance, with high capacity values also at highest rates, and high stability upon cycling. Furthermore, EIS measurements have reveal that the electrode interfacial stability is more compromised at high temperatures. The XAS results have allowed to obtain important information on SEI formation and evolution upon C-ZFO electrodes.

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Role of Metallic Cations in the Crucial Selective Olefination Step of the Synthesis of a New Class of Anticancer Agents

Piermattei P.[1], *Bisconti L.*[1], *Giorgi S.*[1], *Lupidi G.*[1], *Zuccatosta F.*[1], *Marcantoni E.*[1]

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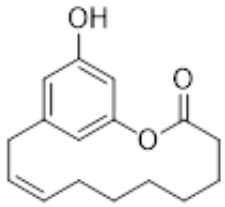
The synthesis of alkenes with a well defined geometric configuration is a continuous challenge in the synthesis of many natural products and drugs[1], for this reason different methodologies have been developed. The Wittig reaction and related transformations for its high level of geometrical control have become the most frequently employed[2]. The counter ion of the base used can be choose in order to obtain different stereoselectivity in Wittig reactions[3], and in recent years, our efforts are focused on the study of the presence of cerium for a better selectivity towards the formation of (Z)-alkenes. The biological activity differences between geometrical alkenes could be partly attributed to different interatomic distance between group that are essential for the activity[4,5]. For this we optimized the methodology of the Wittig olefination in order to applied it in the synthesis of the 1,4-membered macrolide 1 containing a (Z) carbon-carbon double bond and an aromatic moiety fused in the macrocycle. All these features are present in many biologically active compounds[6], but it is rare to find all together in the same molecule. The procedure allowed us to avoid RCM reactions, that use the most toxic transition metals, expensive catalysts, and limit the scale up of the reaction.



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From TiO_2 and Graphite to Graphene doped TiO_2 for visible light photocatalytic degradation of refractory dye.

Rommozzi E.[1], *Giovannetti R.*[1], *Zannotti M.*[1], *D'Amato C. A.*[1], *Ferraro S.*[1], *Cespi M.*[2], *Bonacucina G.*[2], *Minicucci M.*[3], *Di Cicco A.*[3],

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Graphene production is an ongoing challenge for large-scale applications. Many processes are used to produce graphene[1]. Top-down method such as the exfoliation of graphite powder in liquid phase by sonication is a promising route to create high quality graphene in great quantity due to its simplicity, its versatility and its low-cost[2]. Graphene with the thickness of a single carbon atom owns unique physical and chemical properties like large surface area, highly flexible structure, high electrical and thermal conductivity and high chemical stability[3]. With these properties, graphene is an attractive material in applications that require a fast electron transfer, such as photocatalysis. In fact, graphene based semiconductor nanocomposites are considered as good photocatalyst for pollutant degradation[4]. Graphene is an ideal nanomaterial for doping TiO_2 because the formation of Ti-O-C bonds extend the visible light absorption of TiO_2. Furthermore, electrons are easily transported from TiO_2 to graphene nano-sheets and the electron-hole recombination is reduced; this is enhances the oxidative reactivity[5]. In this work, graphene doped TiO_2 nanocomposite was used as photocatalytic materials for the Alizarin Red S degradation in water solutions. Graphene dispersions were prepared by liquid-phase exfoliation of graphite in the presence of a non-ionic surfactant, Triton X-100. The obtained graphene dispersion was characterized by X-Ray Diffraction, Dynamic Light Scattering and UV-Visible spectroscopy and was subsequently used for the preparation of graphene doped-TiO_2 photocatalyst. Graphene doped-TiO_2 nanocomposites showed higher adsorption of Alizarin Red S on the catalyst surface and higher photocatalytic activity for its degradation under visible light irradiation, respect to those obtained with pure TiO_2[6].

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Reflectographic analysis on some paintings at the Pinacoteca of Ascoli Piceno

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A series of diagnostic tests on some paintings by artist Carlo Crivelli[1,2] have been performed. The purpose of this work was to use and combine the results of different non-destructive analytical techniques to improve the accuracy in the determination of the materials used in works of art, which can provide useful information in a complex and heterogeneous situation of studies currently conducted on Cultural Heritage. In particular, the investigations carried out include Multispectral Imaging and X-ray Fluorescence (XRF), which were used to acquire new analytical data concerning the identification of pigments and materials used and the understanding of the modus operandis of the artist. The multispectral system employed was the Hypercolorimetric Multispectral Imaging (HMI), developed by Profilocolore[3]. This approach is based on the measurement of the spectral reflectance, evenly sampled every 100 nanometers, derived as an optimization of the standard colorimetry expanded to a wider spectral range (300-1000 nanometers) and to 7 linear matching functions. This system, allowing to record pixel by pixel an absolute spectral reflectance, was able to discover even little pigment variations (or similarities) not visible to the naked eye. The combination between the information coming from the multispectral system and from XRF allowed to develop a new system of correlation of data coming from different kinds of analysis, to deepen the knowledge about a work of art with the use of techniques that have no impact on it.

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An orthophotographic and multispectral integrated approach at the service of mensiochronology

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Mensiochronology deals with studying the measurements of bricks in historical buildings to go back to their dating[1,2]. The present study shows the development of a methodology to simplify the study of bricks and of mensiochronology, in order to facilitate the measurement procedures, and to refine and expand the results you can get from them. In particular, Hypercolorimetric Multispectral Imaging (HMI) was integrated with Virtual Metric Measurements, made by means of a computer software. This method was applied as a case study to some churches in the province of Macerata, Marche region, Italy. HMI, developed by Profilocolore, is a methodology that allows to measure the spectral reflectance and colorimetry of surfaces in imaging mode with a large spatial resolution (36.3 megapixels images) and spectral reflectance between 300 and 1000 nm. This information is important because both colour and reflectance can be related to the manufacture of bricks[3]. In addition, the image is rendered to an orthophoto: the resulting images show the exact proportional ratio and angular orientation of the original examined surface. This enables to use a metric scale, which establishes the relationship between the number of pixels on the image and the actual size, thus allowing to obtain any measurement from the images taken. We can therefore say that, with the application of this methodology, there will be the great advantage of being able to make measurements with an accuracy comparable to measures made manually, on a much larger surface, with the uniqueness of having at the same time also the colorimetry and a spectral reflectance of the entire surface taken into consideration.

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The "Saint Francis in meditation" by Caravaggio and its twin in Malta: diagnostic analyses

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On the occasion of the exhibition "Francis in the art. From Cimabue to Caravaggio", hosted at the Pinacoteca Civica of Ascoli Piceno (Marche region, Italy), non-destructive diagnostic analyses were performed on many of the paintings displayed. In particular, an interesting comparison between the painting "Saint Francis in meditation" by Caravaggio and a copy coming from Malta was exhibited. Thus, a series of different non destructive and non invasive diagnostic techniques was carried out on both paintings[1]: the aim was to recognize any difference, primarily from a chemical and physical point of view, but also regarding the painting technique[2]. The set of analytical diagnostic techniques employed included: Imaging Spectroscopy (by means of the system Hypercolorimetric Multispectral Imaging, HMI, developed by Profilocolore), Raking Light inspection, Ultraviolet fluorescence, Macro Photography and X-ray Fluorescence. The analyses focused on the most distinctive features characterizing the painting technique by Caravaggio, and this enabled to make a comprehensive non destructive investigation on the two paintings, allowing to detect many differences.

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Development and Analysis of Gelatin-based Bioplastics Coloured with Natural Extracts

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The use of waste by-products from industrial or agricultural processes is a procedure aimed at reducing waste, therefore inherently sustainable. In particular, the production of bioplastics with self-developed procedures, which enter the wider field of DIY materials [1], is a possibility that has the advantage to impede waste dumping, on the other side potentially providing a material suitable for various uses, including commodity objects for everyday use. In this work, a bioplastic based on gelatin, a residual from butchery activities, plasticized with glycerol and water, has been developed with the idea to produce small objects, such as small bowls and costume jewels, which has been coloured using blueberry and beetroot juice. A number of analysis methods have been applied on the obtained materials, especially to evaluate their aging over some period of time, which appears a limitation to wider use of DIY bioplastics so far [2]. The techniques used, which provided some evidence of material degradation over time, included optical microscopy observation, stratigraphy, thermogravimetric analysis (TGA) and UV ageing evaluated using modification of FTIR spectra. Specifically the structure of the bioplastic was studied by ^{13}C CPMAS NMR spectroscopy. Future work would involve starting some mechanical and structural assessment over the obtained materials.

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A New Practical Flow Chemical Synthesis of 3-Alkylidene-2-oxindoles

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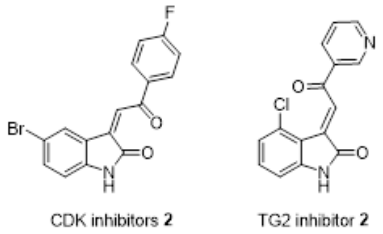
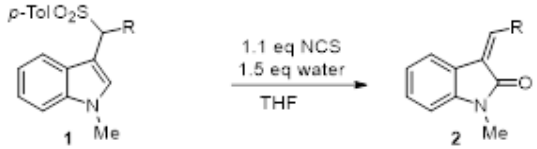
Recently, the synthesis and reaction of 3-alkylideneoxindoles attracted much attention, since this type of compounds are embedded in a number of biologically important molecules and also represent a useful precursors for the synthesis of many pharmacological agents, having prominent biological properties, such as antibiotics, analgesics, nonsteroidal antiarthritic drugs, as well as antiangiogenic and antitumoural antagonists. 3-Alkenyl-oxindoles are in fact an attractive template for the discovery of new medicines, and we can count today several compounds, containing this moiety, currently employed in treatment of various diseases. For example, Woodard an co-workers identified a series of selective plasmodial CDK inhibitors 3 while Khosla and co-workers described 3-acylidene-oxindoles such as 3 as inhibitors of human transglutaminase-2 (Scheme 1).[1]



Scheme 1.

Our approach entails the oxidative conversion of sulfonyl indoles **1**[2] using NCS under controlled conditions using the flow chemistry technique (Scheme 2).[3]



Scheme 2.

This procedure allows the direct formation of alkylidene oxindoles 2 avoiding other by-products arising from over-oxidation of the substrate.

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Design, synthesis and biological evaluation of chemical swiss tools to treat tumors

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Polydentate nitrogen-containing donor ligands derived from poly(pyrazol-1-yl)methanes bearing organic functional groups on the bridging carbon have recently attracted considerable attention and their coordination chemistry towards main group and transition metals have been extensively studied. We have synthesized three carboxylated heteroscorpionate ligands, $[HC(CO_2H)(pz^{Me2})_2]$, $[HC(CO_2H)(pz)_2]$ and $[HC(CO_2H)(tz)_2]$ and we have studied their coordination chemistry towards copper(II), copper(I) and silver(I) acceptors. We have also investigated the use of nitroimidazole (2-methyl-5-nitro-imidazole) as biomolecule to link to scorpionate ligands, as nitroimidazole conjugates of bis(thiosemicarbazonato)copper(II) showed additive or synergistic selectivity for tumor hypoxia compared to their individual components. In particular, we designed two new nitroimidazole conjugated heteroscorpionate ligands, 2,2-bis(3,5-dimethyl-1H-pyrazol-1-yl)-N-(2-(2-methyl-5-nitro-1H-imidazol-1-yl)ethyl)acetamide (L^{MN}) and 2,2-bis(1H-pyrazol-1-yl)-N-(2-(2-methyl-5-nitro-1H-imidazol-1-yl)ethyl)acetamide ($L^{MN'}$), useful for the synthesis of novel copper(I) and copper(II) derivatives to be evaluated for their cytotoxic activity.3 The ligands $[HC(CO_2H)(pz^{Me2})_2]$ and $[HC(CO_2H)(pz)_2]$ have also been functionalized with the potent NMDA receptor antagonist (6,6-diphenyl-1,4-dioxan-2-yl)methanamine, which showed a significant cytotoxic activity on MCF7 human breast cancer cell lines, highly expressing NMDA receptors.4 Some new copper(II) complexes as well as the corresponding uncoordinated ligands were evaluated for their cytotoxic activity towards a panel of several human tumour cell lines.

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Characterization of Additives to Be Used in the Production of Polyurethane Enamels

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In the field of materials a large segment it is represented by polymeric materials. Discovered relatively recently, it was immediately realized their great value from the application point of view. The paints and enamels are among polymeric products, are in fact composed of polymer chains of various kind (PE, PA, PEI, PAI, PU), but at a lower molecular weight[1]. An application of paints and varnishes is the electrical insulation, they are in fact applied on copper wires to allow its use in various electrical and electronic mechanisms. The enamels (Figure 1) of this type are very often compounds, made not only of the polymer matrix (certainly present in greater proportion) but also by various kinds of additives of various nature[2]. The additives are added to the mixture of the crude product and have different tasks, including: increase the properties and then the desired performance of the final product; catalyze the polymerization process both in the production phase that in the enameling one; improve adhesion on the wire; lower the cost of the product. Our research, led along with the group ELANTAS Europe Srl, has been focused on one of these additives, a catalyst, which is used for the polyurethane enamels. This catalyst is actually a mixture of organic molecules, obtained by the condensation reaction between an amine and an aldehyde[3,4]. The purpose of our study was to identify the structures of the above mentioned molecules and also the concentration of these within the same mixture, making use of instruments such as GC-FID, GC-MS, HPLC-MS and HPLC with UV detectors.

Figure 1. Enamelled wire properties

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Computer Science

Understanding Production Chain Business Process using Process Mining: a Case Study in the Manufacturing Scenario

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In a competitive global market where customers are increasingly demanding and laws and regulations continuously change, companies need to adapt rapidly to new conditions in order to advance. A better understanding of the way to work is needed, this was a real need of a manufacturing company that produces coffee machines and sells them worldwide. In particular, the company aims to understand and then improve the production processes. To do that we propose the use of process mining techniques1[1]. We conduct a benchmarking of five process mining algorithms to choose the most suitable for discovering the real production process in the given manufactory scenario. The selected algorithms are: aalgorithm2[2], Heuristics Miner[3], Integer Linear Programming Miner[4], Inductive Miner[5,6] and Evolutionary Tree Miner[7]. Such algorithms were applied to a large log set, concerning six years of production, and then evaluated according to specific quality criteria: fitness, precision, generalization and simplicity. We conclude that the Inductive Miner algorithm is especially suited for discovering production chain processes in the context under study. The application of process mining gives the company a comprehensive picture of the internal process organization. Discovered models were used by the company with successful results to motivate the discussion on the need of developing a flexible production chain. The comparison results are consistent with those of other studies available in the literature[6,8].

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Exploiting multitenancy in cloud applications using patterns

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Multitenancy is the new property of cloud computing that changes the way to develop software. Multitenancy, within the software architecture community, is usually referred to the ability to serve multiple organizations through one instance of a software product and it can be seen as an high level architectural pattern in which a single instance of a software product is hosted on the software vendor's infrastructure, and multiple customers access the same instance [1]. This concept consists in the aggregation of different users, called tenants, in a single instance in contrast with the classic single-user (single-tenant) concept. A tenant can be seen as a closed group of users or a single customer, which is usually charged and handled as a single entity. The aim of multitenancy is the reduction of costs for deploy and maintenance in cloud applications delivered as Software as a Service [3]. To do this, applications need an high configuration level in order to satisfy the requirements of each tenant. In this work we present a list of patterns [2] that enable legacy application to handle multitenancy in a cloud setting. Each pattern is focused for a precise characteristic of an application to cover different customization perspective: Data Configuration, Roles Management, Workflow Management, Process Management, Report Management, and Business Rule Management. For each one, we specify the problem, the context in which the patterns apply, and a possible reengineering of the legacy application to handle the problem. Pattern validation was done through the use of surveys proposed to developer and to other industry experts. This research is related to the Open City Platform project (OCP project, SCN 00467, http://www.opencityplatform.eu/) founded by the Italian Ministry (Ministero dell'Istruzione, dell'Universita e della Ricerca) in the Smart Cities and Communities and Social Innovation initiative.

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BPMN Formal Semantics Implementation in Maude

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Many different languages and graphical notations have been proposed to represent Business Process (BP) models. Among the various proposal BPMN 2.0 standardized by OMG [1] has acquired a clear predominance. BPMN success comes from its versatility and capability to represent BPs with different levels of detail and for different purposes. In defining the notation, OMG did not intend to provide a rigorous semantics for the various graphical elements; instead the meaning of BPMN elements is given using natural language descriptions, allowing for a wider adoption of the notation in different contexts. However, the absence of a formal specifications leaves room for ambiguity about its semantics and it does not allow for formal analysis. In [2] we contributed providing an operational semantics for BPMN in the Structural Operational Semantics style by relying on the notion of Labeled Transition System. As a further contribution, we extended the proposed BPMN Operational Semantics and we implemented it in Maude [3]. Maude is a high-level language and high-performance system supporting both equational and rewriting logic computation [4]. The Maude implementation allows us to simulate the execution of a BP and to verify some properties using the Maude Linear Temporal Logic model-checker. The final result of our work is a toolchain that links together: the Eclipse BPMN Modeler, the defined BPMN Operational Semantics, and Maude. This toolchain enables the formal analysis of BPs.

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Mechanism Design Approach for Energy Efficiency

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In a real world, there exist different energy sources that provide the required energy (photovoltaic (PV), nuclear, hydroelectric, etc). Therefore, the trend of the amount of available energy is constantly changing by the day. At the other hand, the consumption of a community of users depends on users' lifestyles, day of the week, season, ecc. In the literature, this kind of problem is called demand side management (DSM), that is the modification of consumer demand for energy through various methods such as financial incentives and behavioral change through education. During my research activities, I am developing a model that is able to manage the energy demand in order to reach an efficiency goal: consuming the whole produced energy. The model takes into account the social goal that is represented by the optimal use of the energy produced. This can be achieved by behavioural changes induced in the users modifying dynamically the energy cost per hour. In this work, I want to deploy a game-theoretic approach in order to tackle this DSM issue. The objective is to modify users' behavior in order to avoid consumption peaks and to involve the users into a more careful energy consumption. The mechanism will be able to drive users in shifting energy consumptions, by selecting an appropriate energy pricing scheme considering the amount of available energy according to the energy consumption preference of every users. This result could be achieved through an incentive approach, for instance to give more expensive energy rate for specific peak hours. The aim is to develop a mechanism (in a game theoretic sense), that want to pursuit a global objective (the optimal energy use) through the independent maximization of single user's utility, according to the definition of a social choice function and a payment scheme.

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SDN-Based Resources Monitoring to Improve Security in Cloud Computing Scenarios

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Software-Defined Networking (SDN) is an innovative approach to programmable networks that was able to attract more attention during the last years. In the cloud computing scenario, SDN is the key technology that can provide a strong mean to improve its manageability and scalability [1]. SDN is built on the separation between the control and data planes: while the first one encloses application and control layers, the second one represents the network infrastructure layer. However, this separation sends up security red flags when considering the consequences of its adoption. New open issues are introduced [2] and among them, our efforts are focusing on scalability and security aspects. The idea is to use the analysis of resources monitoring and, thanks to SDN features, to provide a reactive system based on the following three keywords: business continuity, self-optimization and auto-healing. We are developing a prototype, based on the definition of proper policies, in order to empower a policy engine which will be able to take decisions and, in real-time, actually provide mechanisms for fast reaction to operational problems. This not only to guarantee business continuity, but also to provide specific auto-healing mechanisms able to mitigate current issues affecting cloud computing scenarios. To clarify a bit better the potential features of the framework, some examples of corrective actions might be: network configuration or reconfiguration, virtual machines (VMs) migration or reconfiguration, or storage commitment. Nevertheless, corrective measures will take into account specific scenarios where mobility must be preserved. Moreover, about what concerns large network attacks, such as Denial of Service (DoS) or distributed ones (DDoS), a fast detection of them can introduce to a flexible control structure to allow fast and specific attack reaction by the framework will evaluate and eventually perform some activities to face distributed attacks.

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A Comparison between Trust Management Models in Cloud Computing

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Over the past few years, cloud computing has been widely adopted as a paradigm for large-scale infrastructures. In such a scenario, new security risks arise when different entities or domains share the same group of resources. Involved organizations need to establish some kind of trust relationships, able to define appropriate rules that can control which and how resources and services are going to be shared. This allows also to boost consumers' confidence in cloud services, promoting its adoption. Establishing trust with cloud service providers (CSPs) supports to have confidence, control, reliability, and to avoid commercial issues like lock in. Among the different surveys in the literature [1] [2] [3], our approach presents a different, simplified classification aiming to reduce the topic complexity, in order to provide a high-level analysis. We categorize, describe and briefly analyse trust models upon the following groups: (i) Policy Based; (ii) Recommendation Based; (iii) Reputation and Feedback Based. We decided to simplify the classification, avoiding complexity and ambiguity while categorizing specific trust models that might belong to different groups, as it usually happens with some hybrid models. However, a small overview is also reserved to biological techniques for defining trust models, since they are gaining some attention in the literature. Cloud computing still presents trust issues as an ambiguous area, representing a barrier to cloud adoption for particular real cases. A higher trust can attract customers that currently are avoiding cloud solutions because they are afraid for their data and seeking a greater confidence level. The lack of a commonly reliable and efficient trust evaluation system is to consider a major issue. Several trust models have been discussed, but what is missing is some accepted criteria to evaluate the effectiveness of such models for a cloud computing scenario.

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Reversible Graph Grammar for RNA

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Graph rewriting formalism is widely used for modelling the dynamics of complex systems in direct and intuitive way. It has been used in computational biology in different contexts, such as RNA tertiary structure motifs encoding[1] and biochemical systems modelling[2]. Besides, in our previous work, we have shown how double pushout (DPO) graph rewriting is used to model the RNA folding as a self adaptive system within S[B] paradigm[3]. Accordingly, the graph transformation encodes simultaneously the RNA functional behaviour and its structure. DPO rewriting rules are applicable whenever the application conditions (identification conditions and dangling conditions) and negative applications conditions are satisfied. The specified conditions can also be used to ensure the reversibility characteristics of DPO. The reversibility of DPO rule has been applied to model dining philosophers problem[4]. Since DPO rules are guaranteed to be reversible (backtrack), we can perform the admissible rewriting rules to model the folding and unfolding pathways of RNA. The backtracking mechanism backtracks out of the dead-ends by undoing all effects of graph rewriting sequences and by selecting the remaining possible rewritings to derive all the possible RNA secondary structures. In this study, as extension of our previous work[4], we introduce reversible graph grammar to formalize and complete the definition of the B and S levels of the S[B][5]. The B-level is represented as a label transition system (LTS) in which the sate space represents the entire folding evolution of the given RNA molecule. The structural level S, represented as a state machine which controls the adaptation dynamics of the B level towards the lowest minimum free energy secondary structure based on state and transition constraints.

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A Formal Approach to Decision Support on Mobile Cloud Computing Applications

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Mobile Cloud Computing (MCC) [1,2,5] is an emergent topic growths with the explosion of the mobile applications. In MCC systems, application functionalities are dynamically partitioned between the mobile devices - which face obstacles related to network, CPU load and storage - and the cloud - a wired infrastructure that provides much greater computing resources than those offered by a mobile device. The main research direction in this field aims at optimizing different metrics, like performance, energy efficiency, reliability and security, in a dynamic environment in which the MCC application is located. Optimization in MCC refers to taking advantages from the offloading process, that consists in moving the computation from the local device to a remote one. The biggest challenge in this aspect is to define a strategy that is able to decide when offloading and which part of the application to move. This technique, in general, improves the efficiency of a system, although sometimes it can lead to a performance degradation. To decide when and what to offload, we propose a new general framework supporting the design and the run-time execution of applications on their own MCC scenarios. It provides all the useful instruments to describe a MCC scenario, including all the parameters that affect the final optimization metric results. In particular the framework provides a new specification language, called MobiCa [3], equipped with a formal semantics that permits to capture all characteristics of a MCC system. Besides the optimization strategy achieved by exploiting the potentiality of the model checker UPPAAL [3], we propose a set of methods for determining optimal finite/infinite schedules [4]. They are able to manage the resource assignment of components with the aim of improving the system efficiency in terms of battery consumption and time. Furthermore, we propose two optimized scheduling algorithms, implemented in Java, based on the exploitation of parallel computation in order to improve the system performance.

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On Avoiding Erroneous Synchronization in BPMN Processes

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Nowadays the importance of modeling organization processes using well-established notations is more and more recognized. In this respect, several notations have been proposed and BPMN [1] has acquired a clear predominance in the last years.

Its semantics is informally given in terms of a token game, where the flow of tokens among the various elements of the model represents the progressing of the corresponding process behavior.

Even though the specification of the notation is semi-formal, in some cases it is important to clarify the behavior introduced by a modeled process. In particular it is important to guarantee the correctness of a model, i.e. avoid undesirable effect not respecting the intention of the designer. For instance, ambiguities can arise in process models including concurrent behavior, where erroneous synchronization can occur. Such a kind of processes generally include sequence flows that can be activated more than once at the same time, referred as unsafe processes.

Our work addresses this synchronization issue by means of a way to recognize the possibly affected models and by introducing additional elements to regulate the synchronizations. Specially, avoidance of erroneous synchronization is achieved using tokens with identity. Future works include a refinement of the process characterization in order to possibly derive a necessary and sufficient condition for safeness, the automation of the placements of the new introduced elements, and working on a plugin for the Eclipse BPMN Modeler [2] which allows to integrate the new elements into the already defined syntax.

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Defining Policies for Management Strategy Evaluation in DISPAS

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Management Strategy Evaluation (MSE) [1] is a simulation technique useful to determine whether a harvest control policy might be successful or not. It uses data collection schemes and control policies in order to generate simulations. The analysis of simulation results will determine which policies are more suitable for the decision makers or the stack-holders aims. MSE evaluates the harvest control rules for a particular fishery. DISPAS [2] is an agent-based simulator for the fish stock evaluation, validated for the stock of common sole (Solea solea L.) in the Northern and Central Adriatic Sea. In this work, we extend the capabilities of DISPAS in order to support MSE. We start by transforming policies into a proper set of parameters that can be introduced as part of the simulator. For example, consider policies based on the parameters of the catch rate (C),

$$C = q * E * B$$

where:

- q represents the catchability, i.e. the efficiency of a particular fishery;
- E describes the fishery effort, e.g. expressed as number of fishing ships and/or as number of working hours;
- B is the total biomass, i.e. the sum of the all fish weights.

The biomass can be calculated at runtime in each time step of a DISPAS simulation. The other parameters can be given by the policy or considered constant. Then, the extended DISPAS will be able to simulate the evolution of the stock given the policy. The results can be analyzed w.r.t. the original aims of the policy makers. For example, the effects on the stock of a policy in which the effort E is doubled can be evaluated by simulating a certain number of years considering a fixed catchability q.

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Developing Spatiotemporal Features of DISPAS 2.0 Simulator

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DISPAS 1.0 [1] is an agent-based simulator that performs the stock assessment of the common sole (Solea solea L.) in the Northern and Central Adriatic Sea. It implements probabilistic monthly-based simulations over time considering an average square kilometer of sea. In [2] the first ideas on expanding DISPAS 1.0 on the spatial scale were put in place by introducing the notion of macro-agents representing the fish population of a certain hexagonal area of the sea located in specific coordinates. Then, the ideas were further developed in [3] by defining a multi-scale simulation model based on the computational model of Complex Automata. This model has been implemented in DISPAS 2.0, the new spatiotemporal version of the simulator, which includes the following features. First, an integration with a Geographical Information System (GIS) was added in order to place each hexagonal agent in its exact coordinates in the Adriatic Sea. The GIS tool permits to perform spatial queries that are used, for example, to define the neighborhood of each agent or to select only the hexagons in which the common sole is present. Second, each agent has been equipped with its own parameters for natural/fishing mortality probability and growth factor. The population of each hexagon is represented as a number of individuals, normally distributed on age, divided by annual cohorts. The population stochastically evolves over time considering the mortality, the introduction of newborns and the input/output due to migration. Finally, a mechanism of communication of agents with their neighbors was developed, which is used, for instance, to correctly implement the migratory flux.

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Talking Hands: a Wearable Device for LIS Translation

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Today in Italy there are more than 100.000 deaf people: their disability relegates them to the fringes of society. Deaf people read the words by deciphering the lips movements of who is speaking. However, they experience great difficulty in communicating because they cannot be understood by people who do not know their sign language. LIMIX Srl and our research group aims to improve the quality of their life.

Our solution is Talking Hands, a device that translates gestures of the sign language into voice. It can interpret the hands movements while a gesture is being made, translate and transfer it to a device equipped with speakers, such as smartphones or bluetooth speakers. Then signs can raise their voice!

The realization of Talking Hands requires advanced skills in electronics for the hardware, math modeling and optimization algorithms for gesture recognition, software and embedded computing for optimized implementation of algorithms and wireless communications of the various components. For this purpose, our research group is composed by mathematics, engineering, electronics engineers and computer scientists from UNICAM, and by business companies already cooperating with the University for a long time. Talking Hands is a tool that will improve the lives of many people, helping their integration in all areas of society by giving them greater autonomy, safety and personal gratification.

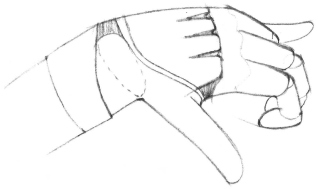

Figure 1: Concept Design of Talking Hands

Epileptic seizures can be anticipated by geometric-topological entropy analysis

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Epilepsy is a complex brain disorder characterized by an hypersynchronous activity of neural ensemble in the brain. Nowadays electroencephalography (EEG) is the golden standard for studying, monitoring and diagnosing epilepsy. Signals (time series), recorded by EEG, represent a description of the dynamics of the brain. Epilepsy is an emergent behavior given by a phase transition between a non-epileptic state (pre-ictal state) and an epileptic one (ictal state) of the neural hypergraph [1-2]. Traditional linear techniques applied to EEG show some limitation to identify these transitions while the non-linear ones seem to be more promising. The understanding of the underlying mechanisms of ictogenesis and propagation requires a suitable formal method to compute the model that supports the anticipation of ictal states. Recently, Topological Data Analysis and topological entropy [3-4], the so-called persistent entropy, are proven to be encouraging for distinguishing healthy from unhealthy patients by showing numerical evidence of the occurrence of phase transitions. We extend the previous work by providing a theoretical justification, based on statistical indexes (skewness and kurtosis), persistent entropy and topological invariants (Betti numbers), of the preliminary numerical results which describe the occurrence of a phase transition; moreover, we also intend to investigate the role of geometric entropy in quantifying the complexity of the networks since a change of complexity is also an indicator of a phase transition [5].

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A formal language for classifying RNA secondary structures

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We introduce a formal language for representing RNA secondary structures as interactions of loops [1] towards a topological shape language [2]. A base loop is an hairpin. All the other loops, such as bulge, helix, inner loop and multiple loop, are compositions of hairpins. Two loops are sequentially connected by base pair weak interactions. We introduce a set of operators to manipulate loops and interactions between loops. The grammar of the resulting language of RNA secondary structure allows us to generate both pseudoknot free and pseudoknotted RNA secondary structures starting from the RNA sequences. Moreover, we can represent a pseudoknot free RNA secondary structure in a "canonical form", thus we have a way to tell whether two given structures differ by a loop. We will investigate the characterization of the higher order language corresponding to the loops interactions [3].

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Implementation of a SPID compliant Identity Provider integrating Shibboleth and CAS

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In recent years more and more services are being implemented as digital services, allowing users to access them from anywhere through the Internet. In this scenario, such services often require a user to be strongly authenticated, meaning that their identity must be unambiguously proved. That's the reason that drove AgID, the Italian agency for digital innovation, to adopt SPID [1], an infrastructure that recently has been introduced into national territory by the Italian law. SPID (Sistema Pubblico di Identità Digitale) aims to bring federated authentication into within the Italian territory, where a trusted Service Provider (SP) delegates the user authentication to an external trusted Identity Provider (IdP), prior to supply a protected resources. This mechanism improves user privacy and security, since the user's digital identity and the relative credentials are verified, safely stored and protected by a trusted entity. Additionally, the user does not need to create a new account in each Service Provider they interact with. Out work aims to develop a SPID compliant IdP. Two software have been deployed into the first attempt to create an IdP that would be appropriate SPID entity: Shibboleth, a federated identity solutions that provides a framework for delegated authentication, and CAS, a web application that performs the actual authentication. Although such systems allows the configuration of some settings, the default deployment is not sufficient to make the IdP compliant to SPID regulation, and further customizations must be developed. So far we have implemented and incorporated three plugins into the software.

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The Value of Patent and Trademark Pairs

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The valuation of patents is assessed with respect to complemental IP strategies, such as trademarks and design patents. I elaborate a novel method and database to gauge the combination of IP strategies regarding the same innovative project, when the patentee pairs the patenting strategy with other formal IP mechanisms. In particular, I analyze jointly the content of legal documents using textual matching algorithms, and I link them with estimates on the premium value of patent protection[1]. I find ample evidences that a pairing strategy based on the combination of patents and trademarks has a large impact on patent valuation with a net increase of about twice the average premium value. The results hold after controlling for several patentee demographic characteristics and patent value indicators typically used in the literature[2]. To interpret these finding I argue on the signaling function of the combined IP strategies. A patent and trademark pair constitutes a signaling device of the high expected value of the underlying invention from a commercial point of view[3].

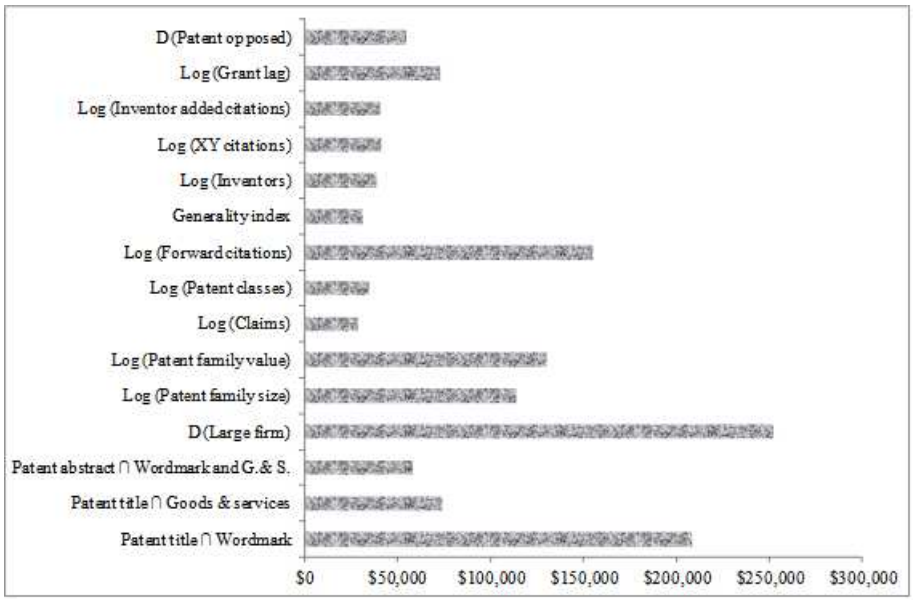

Figure 1: Absolute impact on the patent premium value (in PPP $)

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A comparison of HEED based clustering algorithms - introducing ER-HEED

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A Wireless Sensor Network (WSN) is composed of distributed sensors with limited processing capabilities and energy restrictions. These unique attributes pose new challenges amongst which prolonging the WSN lifetime is one of the most important. Clustering is an energy efficient routing technique that has been widely applied to report data from the WSN nodes to a centralized Base Station. A plethora of different clustering protocols have been proposed. Some protocols are based on equal sized clusters while others use clusters of unequal size. Some others make use of rotation techniques to reduce the amount of cluster head elections. When different clustering approaches are presented different simulation settings are used. In this paper we perform a comparison study of HEED based clustering protocols that are HEED, UHEED, RUHEED and a novel variation of R-HEED that is ER-HEED. We have considered the same network model, the same energy consumption model and we have compared the lifetime of the protocols by considering various case studies. Our comparison study shows the selection of the protocol to be used depends on the case study and the WSN lifetime measure that is considered.

Index Terms-Wireless sensor networks; Clustering protocols; Energy efficiency;

Geology

Studying the soil: from the school organic garden to the IBSE activity in the classroom

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The Farming Soil is the focus of this project which is part of a PhD project on Teaching Earth Sciences at UNICAM. The project has been proposed to the schools with a year long experimentation, in collaboration with the teachers and 120 pupils. The choice to treat the topic of the "farming soil" stems from the awareness that soil is a limited resource which must be protected. It provides food, fuel, fiber and medical products, supports and protects life. It is essential for biodiversity survival and ecosystems, is the largest terrestrial carbon reservoir, stores and filters the water and helps to cope with floods and droughts due to its natural resilience. A renewed interest for agriculture is recently attracting young people, looking for a job or willing to carry on the production of family crops. The school students are therefore exposed to the topic of agriculture, especially in the Marche region, and "the soil" is a topic of interest for both primary and middle schools. The project has been divided in two parts: the first one is for the younger students (6-10 years old), where the didactic activities rotate around carrying out the making of organic garden; in the second part, IBSE (Inquiry-Based Science Education) activities for the older students (11-14 years) have been realized. Classroom activities have been carried out as following: in the first meeting, an individual pre-test is administered; in the second and third meetings, IBSE activities on the farming soil are performed; in the fourth meeting post-test groups is carried out; in the fifth meeting an individual re-test is fullfilled (after 2 weeks from the forth meeting). The activities are organized using the cooperative learning. The IBSE approach [1,2] stimulates the formulation of questions and actions to solve problems and understand phenomena. The data collected evidence that the topic is particularly useful to attract the attention of the younger children. The labs proposing multidisciplinary activities allow to connect several subjects, influencing positively the learning outcomes. For school students of these ages, studying the soil with day by day activities, is an important stage of learning which requires the understanding and of a complex interdisciplinary ecosystem.

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Mineralogical and petrological study of municipal solid waste bottom ash: comparison with volcanic products

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A comparative petrological study of municipal solid waste (MSW) bottom ash, products of incinerators combustion, with natural volcanic products has been experimentally conducted. Preliminary studies were carried out under atmospheric pressure at 1000°C, 1050°C, 1100°C and 1200°C and different melting times from 1 to 72h. The aim was to better constraint the equilibrium reaction time for such compositions, with particular interest in the behavior of Cl and volatile metals such as Pb and Zn. Further experiments were performed in cold seal pressure vessels at 25, 50, 75, 500 and 1000 bars. The waste products consist mainly of polycrystalline rock-like fragments, glass, silicate minerals and various waste metals. In order to characterize and model the bottom ash petrogenesis, all the MSW were mineralogically and chemically studied by using X-ray diffraction, optical microscopy and electron microprobe analyses. Many volatile metals, e.g. zinc and lead, were found to be incorporated in salts and silicates and even in silicate glasses. Their speciation in melts and crystals in municipal solid waste products are still widely unknown. Therefore, this study is important for a direct comparison to natural rock system and, more specifically, to high-temperature volcanic system. Such knowledge can give a more complete understanding of the complex conditions of combustion, melting and crystallization[1]. The glasses here investigated result to be similiar to trachy-basalt but with a more complex heterogeneous glass chemistry. This work will be useful to infer the same results in analogue natural volcanic products and to improve their comprehension.

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Climatic characterization of Ethiopia

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Several papers have been published on different issues regarding the climate of Ethiopia or of part of it. This study attempts to revise the knowledge of such a fundamental feature for local development by means of updated and longer time series, also taking into account a larger number of meteorologic stations than previous studies. Basic climatic parameters such as temperature, rainfall, relative humidity, wind speed and direction, evapotranspiration and aridity have been considered for each available station and their spatial distributions analyzed. The main results of such elaborations have been regionalized by means of statistical and geostatistical interpolation, also taking into account topographic and geographic variables, obtaining several rather detailed (considering the huge extension of the study area) climatic maps. Then, the above climatic parameters have been used to update the Köppen-Geiger climatic classification of the Ethiopian territory too. Climate change is a very important issue with huge repercussions on agriculture and hence on the social and economic development of the Country. Trends of temperature and annual, spring and summer rainfalls have been interpolated for the last decades; temperatures generally show a marked increasing trend, especially for their minimum values, whilst annual rainfalls tend to decrease, with the spring small rains (belg) decreasing at faster rate than the summer more intense ones (kiremt).

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Analysis and classification of physical environment aimed at urban planning: the case of Ancona

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The physical environment plays an instrumental role in determining the spatial distribution of strength and weaknesses (and opportunities and treats) to be taken into account for adequate urban planning and territorial governance. Therefore, within the framework of the UniCam FAR "QLand - Qlife" project (PI Prof. M. Sargolini) an extremely simplified classification of natural hazards and resources has been elaborated and experimented for the urban area of Ancona, aiming at furnishing an extremely valuable tool for both planners and stakeholders. We decided to base all the analyses on publicly available data having an acceptable homogeneity. For natural hazards, we have individuated eight categories: floods, mass movements, soil erosion, coastal erosion, seismic shocks, climate, volcanic activity and glacial-periglacial (the latter two lacking in the study area). All the potentially dangerous phenomena (independently from their typology) have been classified according to three levels of hazard (high, intermediate and moderate); in turn, each of these three classes have been split into two subclasses, according to the possibility to recover or reclaim the threatened area. For natural resources we have individuated six categories: water, sea/lake, landscape, climate, geothermal and mineral (the latter lacking in the study area). Following a logic similar to that applied to natural hazards, resources (once more independently from their typology) basing upon their relevance have been classified into two classes (high and moderate), in turn split into subclasses depending on their exploitability. To allow an easy interpretation of the resulting map, we adopted solid colors to represent hazards, overlaid by hatchings representing resources, thus producing a single synthetic map that can be efficiently adopted as a very useful basis for both urban planning and territorial management. All the above procedures were carried out basing upon digital maps in a GIS environment (ESRI ArcGIS ArcInfo).

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Debris flows and precipitations in the Sibillini Mountains (Umbria-Marche Apennines)

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During the last decades, debris flows progressively frequently occurred in high relief areas all around the world, thus arousing general interest to scientific research aimed at a better understanding of these mass movements. Their often catastrophic impact on artifacts and buildings has also highlighted their relevance for territorial planning. Debris flows need a peculiar combination factors to move: in fact, pore saturation, morphometric features (such as slope angle and thickness of debris cover) and geotechnical parameters of the involved material (such as permeability and shear strength) are instrumental in conditioning rupture and propagation of debris flows. In the Umbria-Marche Apennines, these phenomena have not been thoroughly studied and only recently their dynamics has been taken into account. The Sibillini Mts. area (where the highest peaks of the Umbria-Marche Apennines are found) has been investigated aiming to describe some parameters driving the occurrence of these fast landslides. This has been achieved through detailed geomorphologic survey, sided by climatic studies and GIS based statistical analyses. Historical researches have been carried out too in order to define the space and time framework of these phenomena. To individuate the triggering thresholds for the surveyed debris flows, the spatial and temporal variations of precipitation regime have been particularly investigated, defining their trends. Hopefully, this study will be instrumental for an adequate governance of mountain areas, also leading to reduction of natural risks.

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Spatial distribution of precipitation for the 1981-2010 time span in the mountainous Isonzo-Soca basin (Western Slovenia)

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The hydrographic basin of the Isonzo-Soca River shows peculiar climatic, geographic and physiographic features, resulting the area with the highest total precipitation of the whole southern side of the Alps (cumulative annual values range from 1400 to more than 3500 mm). Since its climatic characteristics still are not very well known, an analysis based upon the data collected in 24 recording stations for the 1981-2010 time span has been carried out. In order to improve the regionalization of data (mostly along the borders), more than twenty neighboring stations have been taken into account too. Statistical analyses of the relationship between precipitation (featuring relevant variation even within short distances) and single topo-geographic parameters did not highlight any significant relation: namely, no really sound relation seems to exist between precipitation and altitude, even though the highest values are typical of mountain areas. To achieve more reliable results, a denser network of recording stations would be needed, mostly for high elevation sites. K-means cluster analysis evidenced that the area can be split into four sectors, while stepwise multiple linear regression highlighted that the distribution of precipitation is related with some local topographic parameters, such as the distance from the valley head, the height of the divide and the aspect of the valley.

Evolutionary trend of the beach of the "Sentina" Natural Reserve (S. Benedetto del Tronto, Marche Region)

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The "Sentina" Natural Reserve stretches itself for some 1.7 Km along the southern end of the littoral belt of the Marche Region, touching the Tronto river mouth. It features typical humid habitats and hosts one of the few coastal dune systems still preserved in the Region. Its beach is still natural, even though it is sided to the south by the more than 300 m long pier, built starting from the left side of the river mouth, and to the north by a very long series of emerged barriers. Both these structures severely influence the evolution of the studied beach, inducing strong erosion with subsequent fast retreat of the shoreline. A systematically monitoring of the area (carried out starting from year 2000 following densely spaced transversal transects along the emerged beach and using a sonar for the down to a bathymetry of 15 m) allowed us to interpret and quantify morphometric and sedimentological variations of both the emerged and the submerged beach (the latter characterized by a series of sandy bars arranged in parallel with the shoreline). The analysis of the above data, carried out in a GIS environment using SDAS (2) demonstrated that up to 2006 an average retreat of 27.7 m has been recorded, with a maximum of 33.5 m in a central portion (transects 38 to 42) and lower rates at the two extremities (below 10 m); the northernmost end of the shoreline is the most stable, thanks to the "protection" given by the neighboring barriers. Even though in 2008 the beach was artificially nourished with about 10.000 m^3 of sand, during the following years the shoreline retreated with an average rate of nearly 4 m/y. We have estimated an average net backing of some 50 m in twelve years, also resulting in the loss of about 42.000 m^2 of coastal dunes. It is therefore logical to infer that, standing the very low solid load of the Tronto River (1), if no intervention is carried out in a few years all the (small) still preserved dune system will be completely destroyed and most of the humid area at its back will be threatened by sea ingression during the most severe storms.

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Historical evolution of shorelines in relation with man-made interventions: the southern Marche area.

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The historical evolution of the southern Marche shoreline (between the Conero promontory and the Tronto River mouth) has been investigated comparing it with both natural and anthropic changes. The study started searching, georeferencing and digitizing in a GIS environment all the available historical maps and the observations deriving from archeological and documental findings, in order to reconstruct the position of shoreline at different times, mostly for fluvial mouths. It allowed us to highlight that, at least for the last two millennia, anthropic interventions influenced coastal dynamics more than natural (climatic) changes. In fact, for all the investigated sites it clearly emerged a close relation between shoreline fluctuations and forestation/deforestation processes carried out in the hydrographic basins. Among others, it emerged that river mouths progradation continued up to 1930, well after the end of the "Little Ice Age" (around 1850). The above relation is particularly striking for the last two centuries, for which we have both quite accurate maps and census of forested areas. During the XIX century, notwithstanding the warm climate favored slope protection, widespread deforestation resulted in a regular advance of shorelines (average rate about 4.95 cm/y for the first hal of the century and 1.08 m/y for the second half. The XX century featured a more irregular behavior with substantial retreat after the '30s: this derives almost exclusively from anthropic interventions in the river basins (construction of dams, river bed quarrying, river reshaping, abandonment of crops etc.) leading to a severe decrease of solid load. For the last few decades and at present, the most important factors driving the behavior of coastlines resulted to be the various interventions carried out along the beaches and in front of them to reduce erosion.

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Reconstruction of the geological evolution and stratigraphic architecture of late Quaternary continental deposits through field and boreholes data in the lower Chienti River basin

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The reconstruction of late Quaternary stratigraphic architecture along present coastal and river plains is instrumental for resource management and hazard reduction, including estimate of water resources, defence from salt intrusion and reliable prediction of pollutant dispersal pathways. To this aim, this paper integrates outcrop and subsurface data to present a high-resolution study of the stratigraphic architecture of the late Quaternary continental sediments within the terminal portion of the Chienti River valley. The study area, located in the external sector of the Marche Region, roughly between the villages of Morrovalle and Villa San Filippo, is characterized by two major hydrographic catchments related to the Chienti River and one of its tributaries, the Ete Morto River. In order to reconstruct the geological and stratigraphic evolution of terminal portion of the Chienti river, two main datasets have been used: the 1:50,000 scale 303-Macerata and 304-Civitanova Marche geological Sheets and an exceptionally high amount of subsurface data, consisting of 527 boreholes provided by ARPA-Marche. The geological maps were verified on the field, particularly along the boundary between the two sheets, and were digitalized by ESRI ArcGIS ArcInfo 9.1, whereas the stratigraphy beneath the present Chienti alluvial plain was reconstructed along five transects transverse to the valley direction (maximum length about 6 km). Cross-sections highlighted the occurrence of a flight of Late Quaternary alluvial terraces incised into the Lower Pleistocene bedrock (alternations of prevailing pelitic terrains and arenaceous layers) and resulting from at least four episodes of valley incision and infilling, probably triggered by the interplay regional tectonic uplift and glacio-eustatic sea-level fluctuations. The first- and second order terraces are suspended and usually separated by substrate exposures, whereas the third and fourth-order terraces are in continuity and consist of amalgamated fluvial-channel gravels and floodplain silts and clays. The older terraces are tilted more than the younger ones and the basal surface of the fourth-order terrace, the best preserved of all, displays the typical concave-up morphology with some anomalies near the confluence of the Ete Morto in the Chienti River (E-E' section), where a 10 m high threshold occurs.

A microchemical and spectroscopic study of the obsidian from Mt. Arci (Sardinia, Italy)

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The aim of this research is the characterization of the obsidians from M. Arci (Sardinia, Italy), which show an anomalous wide array of textures and colors. The common black color is accompanied at Mt. Arci by red colored samples but also a particular red-black combination, sometimes intercalated one to the other, whose reasons and mechanisms of formation is still to be explained. For this reason a full characterization has been carried out, including optical polarizing microscopy, microchemical composition determinations and infrared spectroscopy analysis. The petrographic analysis shows the presence of a fluidal fabric only in the red/black samples whereas the black samples have less crystals and are more homogeneous. It is also evident the presence of up to three zones in the same sample, characterized by increasing amounts of crystals respect to the ground mass which can be related to the color. The evaluation of the chemical composition by Electron Microprobe Analysis (EMPA) and comparison with data from the literature assign the rhyolitic composition of all the obsidians and document their metaluminous character. FTIR (Fourier-Transform Infra-red Spectroscopy) reveled that the water content ranges from 0.1 to 0.6 wt% and FTIR imaging showed a positive correlation between the water content and the crystal contents. The combined results from these analyses suggest that the visual variability among the studied obsidians is less related to variations in major element chemistry but rather is correlated with the quantity of water and the presence of crystals. Both these characteristics are connected with the nucleation process taking place during the formation of the obsidians, since a small quantity of water in the melt can facilitate crystal formation. This could explain the well defined boundaries between the red/black/colorless parts and the different amounts of crystals in the different zones of the obsidian samples.

Anatomy and facies characterization of turbidite channel fill deposits: The Santa Mara Channel from the Gorgoglione Flysch Formation, Southern Italy

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Here is presented a study focused on the outcrop characterization of a single submarine channel element from the upper Miocene Gorgoglione Flysch Formation in the Southern Apennines of Basilicata, Italy. This formation is a 1,500-meter-thick package of predominantly coarse-grained turbidite deposits which record the filling of a piggy-back basin.

This study focuses on an interval near the town of Castelmezzano which provides a near complete exposure of a single deep-water channel-fill approximately 50 meters in thickness and several hundred meters in width. This channel, named the Santa Maria Channel, after a nearby church, was measured and described in 8 detailed stratigraphic sections spaced several meters apart, providing data for the sedimentological description and correlation of the stratigraphy. Two primary facies associations are described here. The lower association consists of tabular, coarse-grained, medium- to thick-bedded sandstones interbedded with thin, laterally continuous mudstone layers interpreted as frontal lobe deposits.The upper facies association consists of a basal, very-coarse grained, un-bedded, poorly sorted polymictic conglomerate with a coarse sand matrix passing upward into very coarse grained, normally graded sandstones and micro-conglomerates with aligned mud-clast intervals, grading upwards into medium- and large-scale cross-bedded sandstones interpreted as channel fill deposits. The erosional boundary separating these two facies associations shows a complex erosional relationship with several apparent cut and fill events and upward stacking. Analysis of outcrop data was enhanced by the use of Gigapixel imagery and 3D Photogrammetric outcrop reconstructions to gain or more complete perspective on the exposure. This combined methodology is employed as an attempt to improve outcrop characterization, identification of important features, and correlation of stratigraphy using traditional and modern tools.

Integrated Sedimentological and Palaeontological (Pollen, Molluscs, Fishes Foraminifers, Ostracods) Analyses of Middle Pleistocene Palustrine and Lagoonal Sediments From the Peri-Adriatic Basin (Abruzzi, Central Italy)

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Paludal and lagoon deposits hold high sensitivity to environmental changes and, therefore, are key-stratigraphic intervals for studying past and present climate changes. A 15 m-thick outcrop section exposed at Torre Mucchia, on the sea-cliff north of Ortona, eastern central Italy, provides a rare Middle Pleistocene paralic succession along the western Adriatic Sea. An integrated study of the section, including facies and microfacies analysis and characterization of paleo-biological associations (mollusks, fishes, ostracods, foraminifers, and pollen), enabled a detailed reconstruction of the paleoenvironmental and paleoclimatic conditions during Marine Isotope Stage (MIS) 17. These paralic strata form a transgressive succession composed of palustrine carbonates overlain by back-barrier lagoonal mudstones. The palustrine carbonates exhibit some of the typical features (mottling, ferruginous nodules, root traces and mixed terrestrial and freshwater gastropods) encountered in freshwater palustrine limestones deposited within seasonal freshwater wetlands (marl prairies) and were abruptly replaced by a mud-rich barrier-lagoon system. Within these deposits, the faunal assemblages are consistent with a low-energy brackish environment characterized by a relatively high degree of confinement. The pollen record documents the development of an open forest vegetation dominated by Pinus and accompanied by a number of mesophilous and thermophilous tree taxa, whose composition suggests a tentative correlation with MIS 17. The new pollen record from Torre Mucchia improves our understanding of the vegetation development in the Italian Peninsula during the Middle Pleistocene and sheds new light on the role played by the most marked glacial periods in determining the history of tree taxa.

On the ecotrophic role of the giant Neogene shark Carcharocles megalodon: some notes from the Pisco Formation of Peru

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The extinct otodontid shark species Carcharocles megalodon is known by giant serrated teeth and large vertebrae from Mio-Pliocene marine deposits worldwide. Reaching a total body length greater than 16 m, C. megalodon is regarded as an apex predator which likely occupied the top of the trophic chains of the Neogene global ocean. Despite C. megalodon being interpreted as a whale-eating predator, and its fossil remains being common in Neogene deposits worldwide, little direct evidence for the trophic ecology of this mega-toothed shark arose from the fossil record to date. We report on long and serrated shark bite marks attributed to C. megalodon affecting fossil mammalian bones collected from late Miocene shallow-marine deposits of the Pisco Formation exposed at Aguada de Lomas (South Peru). These occurrences, the first in their kind from the Southern Hemisphere, significantly expand the record of bite marks of C. megalodon; moreover, for the first time a prey of C. megalodon is identified at the specific level (as Piscobalaena nana, a diminutive member of the extinct mysticete family Cetotheriidae). Due to the fragmentary nature of the studied material, it was not possible to ascertain if the observed bite marks were due to scavenging or to active predation. Nevertheless, based on actualistic observations and size-based considerations, we propose that small-sized mysticetes (e.g., P. nana) could have been one of the target prey of adult C. megalodon. A predatory behavior somewhat similar to that of the great white shark attacking seals may be hypothesized for C. megalodon preying upon small mysticetes. We suggest that C. megalodon was a generalist apex predator whose trophic spectrum was still focussed on small-sized baleen whales. It is therefore interesting to observe that the extinction of C. megalodon (occurring at the end of Pliocene) roughly coincides with the the decline and fall of various lineages of small-sized baleen whales (including most Cetotheriidae). The disappearance of the last mega-toothed shark could thus have been triggered by the collapse of the archaic diminutive mysticetes (mostly inhabiting coastal upwelling-influenced waters of warm to temperate oceans) in favor of modern gigantic baleen whales (seasonally migrating to high latitude cold waters), the latter event being possibly driven by long-term planetary oceanographic and climatic changes. Acknowledgements. This research was supported by a grant of the Italian Ministero dell'Istruzione dell'Università e della Ricerca (PRIN Project 2012YJSBMK), by the University of Pisa (PRA_2015_0028), and by a National Geographic Society Committee for Research Exploration grant (9410-13) to G. Bianucci.

Geomorphological evolution and human settlement of the Sabaudia lake (Tyrrhenian sea, central Italy)

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This work shows the preliminary results of recent geomorphological and geo-archaeological researches carried out in the area of the Sabaudia lake (also known as Lake of Paola), within the Circeo National Park. This area has very important archaeological goods which includes remnants date back to the early Paleolithic (remains of Neanderthal man, Guattari cave-Mount Circeo) and the Roman Imperial Age. The Sabaudia lake, separated from the Tyrrhenian Sea by a dune ridge up to 27m high, shows an elongated shape parallel to the shoreline. To the east it is characterized by six narrow bays, called "arms" that correspond to valleys incised during the sea level lowering of the last glacial period. The dune ridge that created the wide lagoon system, was created after the sea level rise that reached its peak, according to several authors, after the Holocene climatic optimum (approximately 6000 years BP). Archaeological evidence of pre-Roman age are, however, very rare; therefore further studies are needed to include them in a context of geomorphological evolution before and after the formation of the lagoon. The archaeological remains of the Roman period in the area are of great value and testify an important phase of the urbanization of the lagoon. The Roman harbor and its entrance with parallel jetties (I century AD), located in the extreme southern portion of the lagoon, belongs to the category of Roman canalizations called "fossae", artificially made for port and commercial purpose. The function of this works was to connect the Tyrrhenian Sea with the inner part of the lagoon where the villa of the Emperor Domitian (I century AD) and other relevant works, such as harbors, aqueducts and cisterns are still visible. Recent studies evidenced the presence of two paleosoils within the main dune, next to the entrance of the Roman harbor and both subjected to radiocarbon dating. The oldest paleosoil (calibrated age AD 900 to 1030), with a thickness ranging from 20 to 60cm is covered by approximately 4m of sand up to the top of the dune ridge. The location and the development of this paleosoil seem to indicate the presence of a dune lower than present, with a smooth profile and dipping toward the south near the harbor. In this context, the top of the dune during the Roman period was certainly placed at lower altitudes and, possibly, it was dip to the harbor with a minor slope. Most likely the Roman wall bordering the entrance of the harbor (Opus reticulatum), now completely covered by sand dune, had not functions of protection and kept behind large spaces. This assumption was also supported by geophysical surveys conducted with ground penetrating radar (GPR). The second palaeosoil, younger (calibrated age AD 1,040 to 1,100 and AD 1120 to1260), has been observed approximately 2m above the previous one year and shows comparable thickness and slope. Studies from other authors and field surveys allowed to assume, always in Roman times, a higher extension (even if slight), of the lagoon. Considering the current elevation of the archaeological remains, it is likely to assume that the Villa of Domitian was closer to the shoreline of the lagoon itself.

Teaching Paleontology at school: a focus on fossils with a University-Schools-Museum project

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The aim of this work is to experiment new ways to favour the approach of Paleontology in Italian schools, by making interdisciplinary links between science, history and geography with an approach based on hands-on and fieldwork approaches. The research started with the observation of the minimal role of Paleontology topics in the school textbooks and its nearly absence in the national curriculum for primary and lower secondary school (grades 1-8). However, in spite of the little space devoted to it, the teaching Palaeontology is important as an introduction to multiple scientific thoughts and basic science concepts, as a tool to understand the geological time, the Earth environments in the past and their transformations with time, as a foreword to all the environmental sciences. The project sees the collaboration among school of the Monfalcone area (Friuli Venezia Giulia, Italy), the Museum of Natural History in Trieste and the PhD program on Teaching Earth Sciences at University of Camerino. This collaboration is focused in particular to make aware the students about the paleontological aspects in the areas they live in, after a preliminary meeting with the teachers, during which topics, methods and calendar of the activities are explained. A first presentation of the subject to the students is made, followed by a classroom interactive lab which takes advantage of the well evident local lithologies, used as building materials. The students are invited to look for Rudists or Ammonites in the rocks in the school stairs and windowsills or outside, which prompts many points of discussion. This activity is followed by making fossils models using paper and glue, building three-dimensional models of environments and conditions where they used to live, creating sketches starring these animals. During the lab activities, the students can see and touch original fossils, which helps them make connections and better understand their 3D morphology and the link to the 2D as observed in the school windowsills. Interdisciplinary connections with other disciplines are suggested a Natural History Museum visit and a fieldwork experience in a paleontological area are carried out, followed by the project assessment, the teachers' questionnaires and a final evaluation of the activity. The project (which involved 600 students) lasted the entire scholastic year and was built to give the teachers the competence, in the future, to carry it on in autonomy. Preliminary results evidence a strong interest by the teachers and good learning achievement and skills acquisition by the students.

Recent variations of the nivo - thermic parameters in the territory of the Dolomites and venetian Prealps

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The analysis of recent snowfalls in the medium-high mountain areas of the Mediterranean basin is considered an instrumental tool to evaluate present climatic change. Aim of the study was to define the space and altitudinal distribution of snowfall and temperatures, as well as to outline recent trends, considering the signal defined by similar recent studies in the Alps, which show a general decrease of snowfalls and a significant increase of temperatures. It was therefore considered monthly and seasonal thermo-nivometric data deriving from fifteen automatic measurement stations operated by ARPAV from the second half of the '80s and located at altitudes approximately ranging between 1430 and 2620 m a.s.l.. The parameters analysed were: cumulated height of fresh snow, number of snowy days (with Sh $>$ 1cm), continued snow cover and average air temperature (AAT). In the study area (about 4500 km^2 wide) at elevation about 2000 m as an average about 323 cm of seasonal fresh snow are recorded between November and May; the snow remains on the ground for about 179 days and there are about 44 days with snowfalls (Sh $>$ 1cm). As an average, fresh snow cover increases about 17 cm (and reduces itself to 7.6 cm) for every 100 meters of increasing altitude. The average annual temperature is about 3.3°C, reaching 0°C at about 2800 m a.s.l. The nivometric and thermometric trends show quite surprising evidences; in fact, both for fresh snow thickness and for snowy days there was a general increase - resulting from some recent very snowy seasons - while the persistence of snow on the ground a more contrasted signal is evident. Temperatures show a marked increase (about 1.3°C) in the pre-Alps, while in the Dolomites, temperatures tend to decline (about 0.5°C). Given the particularities of these results, it will be essential to extend the study area to the entire Tridentine mountains, in order to understand if these signals are found at a more extensive scale

Intense Rainfalls and Flooding Problems in the Sea Resort of San Benedetto Del Tronto (Adriatic Sea, Central Italy)

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San Benedetto del Tronto, located in the southern part of the Marche Region along the "Palms Beach", is a very important Italian touristic seaside resort. It faces the Adriatic Sea and is elongated between the Tronto and Tesino rivers along a narrow stretch bounded westward by inactive wave cut cliffs. The climate is sub-coastal Adriatic, with mild winters and low precipitation, temperate summers and never particularly rainy intermediate seasons. The high population density (over 2500 people per km^2) and the complex physiography favor inundations that cause property and image damages during summer (when the number of residents triples) as a consequence of convective intense rainy phenomena. The frequency of these inundations is typically one or two events per year, but during 2012 a number of extreme events affected the town since February. The analysis of precipitation is related to weather conditions causing such extreme events: it demonstrates that short and intense downpours started to characterize also spring months and become more frequent in autumn. Moreover, the development of new climatic-dynamic patterns is observed, deriving from substantial sea water warming during summer. The study includes also a precipitation and temperature characterization for the last two decades and particular attention is paid to the analysis of principal climatic indexes at climatic-tourist level (days of frost, tropical days and nights). Taking into account the results of these analyses, of a new rainwater drainage system was designed and is currently nearing completion. This work has already found extremely efficient in heavy rainfall - over 70 mm in about 18 hours - occurred March 23, 2016

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Mantle dynamics in the Red Sea region

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Understanding geodynamic processes associated with the transition from continental rifting to sea floor spreading is a major challenge in the Earth Sciences since they are still poorly known. The Red Sea is the unique place in the world where these processes can be studied because it shows all the different opening stages of formation of a new ocean. The opening of the Red Sea started 30 Myrs ago as a conseguence of slab pull exerted along the southern Eurasian subduction zone. At the same time the Afar mantle plume started to uplift the Ethiopian plateau. The objective of this reaserch is studying flows that occurred in the mantle beneath the Red Sea region since 30 Ma using a multiprocessor finite elements numerical modelling software designed to solve mantle convection problems, taking into account of plate kinematic constrains and mantle rheology. This approach allows to solve numerically the six governing differential equations for mantle convection, that is, conservation laws of mass, momentum, and energy, and the state equation [1]:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\rho\left[\frac{\partial v_i}{\partial t} + \frac{\partial v_i}{\partial x_j} v_j\right] = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\eta\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) + \lambda \frac{\partial v_k}{\partial x_k}\delta_{ij}\right] + \rho g_i$$

$$\rho c_p \dot{T} - \alpha T \dot{p} = \Phi + \frac{\partial}{\partial x_i}\left(k \frac{\partial T}{\partial x_i}\right) + \rho H$$

$$f(\rho, p, T) = 0$$

where ρ is density, v is the local flow velocity, p is the thermodynamic pressure, η is the viscosity, λ is the second viscosity, g is the gravity acceleration, Φ is the viscous dissipation, c_p is the specific heat, T is the temperature, α is the thermal expansion coefficient, k is the thermal conductivity and H is the radiogenic heat. These equations can be solved for pressure, velocity, density, and temperature starting from a set of boundary conditions and temperature initial conditions. The numerical modelling will be run on a parallel cluster of 64 CPUs available in the Geophysics lab to obtain adequate performance.

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Time and space distribution of precipitation in the Marche Region (Central Italy): preliminary observations.

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The available data collected at 111 rain gauges in the Marche region and in its immediate neighbor during more than fifty years have been regionalized and analyzed separately for the 1950-1989 and 1991-2007 time spans (103 and 100 recording stations, respectively), in order to individuate time variations connected with global climate change. The study area covers about ten thousand square kilometer and belongs to the Adriatic side of Central Italy. Looking at the raw data, it is evident that for both periods precipitation in every month show a marked increase moving from the coast upstream (i.e. increasing the elevation), with a minimum in the SW portion of the region. To interpolate the sparse data, multiple regressions have been calculated (by means of GIS and Statistic packages) using various independent variables derived from a detailed DEM and digital topographic maps: elevation, latitude, distance from the sea, slope aspect, distance from rivers, distance from divide and local relief (i.e. difference of elevation between the divide and the river). The method allowed to describe more than 70The successive step was to individuate and explain the outliers, in order to increase the accuracy of the interpolation. Finally, the resulting mathematical model has been used to regionalize the rain gauge records, thus obtaining fifteen maps: three maps (one for each period and one depicting the difference among them) for annual values and three for each season. Observing them, beside the already said observation regarding the vertical gradient of precipitation, it is possible to notice that recent pluviometric changes are not homogeneously distributed, even though a general trend toward a dryer climate clearly emerges.

Quality Control Of Climatological Time Series In The Province Of Macerata (Adriatic Side Of Central Italy)

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The analysis focused on more than 100 meteorological recording stations located in the Province of Macerata (Marche region, Central Italy) and in its neighbours; it aimed to check the time series of their climatological data (temperatures and precipitations), covering about one century of observations, in order to remove or rectify any errors. It has been done following the general guidelines of the WMO, with some important difference (mostly in the method). Data have been classified on the basis of validation codes (VC): missing datum (VC=-1), correct or verified datum (VC=0), datum under investigation (VC=1), datum removed after the analysis (VC=2), datum reconstructed through interpolation or by estimating the errors of digitization (VC=3). Various checks have been used for each climatological time series:

1. Logical Control - investigating gross errors of digitization (VC=2).
2. Internal Consistency Check - to verify data are out of their climatic zone range (VC=2).
3. Tolerance Test - to compare each datum with the historical record it belongs to; it usually defines only suspect data (VC=1).
4. Temporal Consistency - allows an evaluation of the time sequence of data, setting a specified range for each station basing upon its historical records (VC=1).
5. Spatial Consistency - Data are finally compared with the ones contemporaneously recorded in a set of neighboring rain gauges in order to recode VC=1 as VC=2 or VC=0.

Missing and removed data have been reconstructed through interpolation using co-kriging techniques (assigning VC=3), using database managing software in a GIS environment (ESRI ArcGis ArcInfo). The refused data are 1,286 out of 77,021 (1.67%) for the precipitations and 375 out of 1,821,054 for the temperatures (0.02%).

Structure of Fe- and Co- doped ZnO as anode material for Li-ion batteries

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Transition-metal-doped zinc oxide has gathered significant interest in the scientific community because of its potential for application in spintronics devices. This same material has been recently demonstrated to be also a very promising alternative anode material for Li-ion batteries[1]. Herein, we report a complete structural study of the pristine anode material, $Zn_{0.9}(Fe/Co)_{0.1}O$ nanoparticles prepared through sucrose assisted wet chemical synthesis, by X-ray diffraction (XRD) and X-ray absorption spectroscopy (XANES and EXAFS)[2]. Preliminary results from experiments on Fe-doped ZnO cycled anodes will be also presented. Structural refinement of powder XRD data revealed the absence of reflections related to spurious oxide phases and showed that different dopants or synthesis conditions remarkably affect the average crystallites size. Fe, Co and Zn K-edge XAS spectra showed that both Co and Fe substitute Zn in the host wurtzite structure. From the analysis of the XANES spectra, we found that Co is divalent, whereas Fe is trivalent in $Zn_{0.9}Fe_{0.1}O$, and 95% trivalent in carbon coated $Zn_{0.9}Fe_{0.1}O$. The aliovalent substitution of Fe^{3+} for Zn^{2+} implies the formation of local defects around Fe^{3+} such as cationic vacancies or interstitial oxygen, for charge balance. Indeed, the EXAFS signals measured at the Fe K-edge show features strongly damped with respect to those measured at Zn and Co K-edges in pure ZnO and $Zn_{0.9}Co_{0.1}O$ consistently with the occurrence of structural defects in the immediate environment of Fe^{3+} in tetrahedrally coordinated sites. The influence of the dopant on the highly reversible conversion-alloying lithium storage mechanism of such materials is still not completely understood. Therefore, the herein reported results may enable the further optimization and design of improved and/or new active materials.

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Innovative application of a micro-CHP with geothermal energy and both electrical and thermal storages: a pilot study case in Marche region (Italy). (MATREND project - FAR 2014-15 P.I. Invernizzi)

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The use of Earth's underground is a key factor in the effort to provide economic and safe solutions for the future energy supply. In addition to supply heating and cooling requests and hot water demand both for private and public buildings, energy consumption has started decreasing in the last decade in order to satisfy the European targets proposed by Kyoto Protocol "20-20-20". The exploitation of geothermal resources using Ground Source Heat Pumps proved to be an optimal choice. However, for each Ground Source Heat Pump a considerable amount of electricity is needed during the entire year. In Italy, more than 50% of electricity requests are supplied by fossil fuels' consumptions. Thus the crux of this innovative application is in the selection of a micro-CHP (Combined Heat and Power) i.e. a Solid Oxide Fuel Cell, as a continuous electricity provider, that, despite it uses natural gas, is able to save more than 30% of fossil fuel consumption each year. This innovative heating and cooling system is made up of an electrical energy storage and both a latent (filled with PCM, Phase Change Materials) and a sensible heat storage. This experimental project, adopting a multidisciplinary investigation, is already in place at the Geology Division of the School of Science and Technology of University of Camerino. The main objectives of this research project are: - to optimize the knowledge about low enthalpy geothermal plants, focusing on heat transfer enhancement tested in two experimental geothermal boreholes; - to test commercial and new grouting materials, in particular thermal properties, used to sustain wall boreholes as well as to evaluate the temperature of the underground; - to monitor heating and cooling system performances month by month and to analyze greenhouse gases emissions reduction and operating costs and so economic advantages. The realization of the experimental plant involved several steps: i) general knowledge of geological conditions; ii) drilling of geothermal boreholes; iii) in situ measures of the underground thermal properties; iv) laboratory investigations of thermo-physical properties and mineralogical determinations both of drilled lithologies and grouts (commercial and innovative); v) construction of an innovative hybrid geothermal-micro-CHP heating and cooling system for the department building; vi) monitoring of both PCM performances and this system's adaptability in real operating conditions; vii) measurement of both environmental and economic advantages.

Geothermal circulation in the Tocomar volcanic area (Puna plateau, Argentina): structural control and evidences from geophysical methods

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The reconstruction of the stratigraphic and structural framework, and the hydrogeology of geothermal areas is fundamental for understanding the relationships between cap rocks, reservoir and circulation of geothermal fluids and for planning the exploitation of the field. The Cerro Tuzgle-Tocomar geothermal volcanic area (Puna plateau, Central Andes, NW Argentina) has a high geothermal potential. It is crossed by the active NW-SE trans-Andean tectonic lineament known as the Calama-Olacapato-Toro (COT) fault system, which favours a high secondary permeability testified by the presence of numerous springs. New stratigraphic and hydrogeological data on the geothermal field, together with structural analyses, morphostructural and remote sensing evidences, and associated with geophysical magneto-telluric (MT) surveys are here presented. Our data suggest that the main geothermal reservoir is located within or below the Pre-Palaeozoic-Ordovician basement units, characterised by unevenly distributed secondary permeability. The reservoir is recharged by infiltration in the ridges above 4500 m a.s.l., where basement rocks are in outcrop. Below 4500 m a.s.l., the reservoir is covered by the low permeable Miocene-Quaternary units that allow a poor circulation of shallow groundwater. Geothermal fluids upwell in areas with more intense fracturing, especially where main regional structures, such as NW-SE COT-parallel lineaments, intersect with secondary structures, such as at the Tocomar field. Away from the main tectonic features, as in particuar at the Cerro-Tuzgle field, the less developed network of faults and fractures allows only a moderate upwelling of geothermal fluids and a mixing between hot and shallow cold waters. The integration of field-based , remote-sensing analyses and mageto-telluruc (MT) geophysical profiles at the Cerro Tuzgle-Tocomar area proved to be effective in approaching the prospection of remote geothermal fields, and in defining the conceptual model for geothermal circulation.

Meso- and macro-scale gravity-driven horizons within basinal succession: the case study of Maiolica Formation, Gargano Promontory, Southern Italy

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In this study, we describe intraformational mass transport deposits (MTDs) at various scales occurring within base-of-slope to basin sediments of the Maiolica Formation cropping out in Gargano Promontory, Southeast Italy. The Maiolica Formation, an Early Cretaceous deep basinal succession is represented by undisturbed intervals of flat-lying, thin-bedded, micritic limestone interstratified with intervals of lithologically similar, but structurally distorted beds. Meanwhile the small-scale MTDs are often represented by slides or coherent slumps, the mesoscale MTDs often form a continuum of slides, coherent and incoherent slumps, and debris-flow deposits. These meso- and small-scale MTDs are easily recognized in the outcrop scale, as they represent layers containing deformed beds surrounded by layers of horizontal undeformed strata from bellow and above. Unlike meso-scale MTDs, the largescale intraformational MTDs might be tricky to identify because only few key outcrops can provide evidence of their presence. The large-scale MTDs exhibit many structural elements (such as faults, thrusts, folds, extensional fissures) that can be easily confused with the structural features of tectonic origin. Large mass movements often cause distortion of the overriding strata underneath the transported material and forming a basal shear layer. These layers may appear as simple small-scale MTDs. However, the unidirectional orientation of folds and thrust orientation and folded stylolites are the evidence that the strata within these horizons were at least partially lithified before the distortion. The field observations allowed us to relate the internal architecture of mesoscale MTDs to the distance along the downslope movement. Moreover, we were able to distinguish superficial from deep-seated deformation horizons and to propose the model of large-scale gravitational events along the paleoslope of the carbonate platform.

Experimental study of monazite solubility in granitic melts

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Monazite is one of the most important rare earth elements (REE) minerals and occurs in granitic/rhyolitic rocks with compositions ranging from peraluminous to peralkaline. It can also be a significant host for geochemically useful elements such as U and Th, and it can serve as an indicator of magmatic temperatures and petrogenetic relationships in silicic magmas. The stability of monazite can affect the behaviour of REE and plays the dominant role in controlling REE abundances in felsic magma suites. The behaviour of rare earths in felsic systems has considerable economic importance, as some of the most important rare earth deposits are related to granites [1].

In the frame of more general work aimed at studying geochemical behaviour of REE in different granitic magmas, we have determined monazite saturation and solubility in a series of synthetic silicate glasses of granitic composition. The solubility of synthetic La-monazite ($LaPO_4$) and Ce-monazite ($CePO_4$) in hydrous haplogranite-based peraluminous to peralkaline melts was determined at experimental conditions from 750°C to 850°C, l kbar to 2kbar, water saturated conditions. Three sets of high temperature 1 atmospheric experiments wer°e done for each composition ($HPG8_{0.9}$, $HPG8_{1.5}$, and $HPG8_2$, where subscripts indicate molar alkali/alumina ratio) at 1400°C. Major and minor elements analyses were determined by electron microprobe. Monazite solubility strongly increases with the peralkalinity of the melt, similar to previous observations concerning apatite and zircon solubility. Microprobe analyses show that the solubility of both Ce and La monazite depends strongly on temperature and melt composition and is especially low for peraluminous compositions, and highest in peralkaline compositions.

GeoQuest VESUVIUS a Class Role Playing Game

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The aim of the work is to use the latest ICT techniques to create innovative educational products. GeoQuest Vesuvius is a class Role Playing Game to teach Earth Sciences, History and Mythology all together in a unique interdisciplinary approach. The game seems to be a perfect vehicle for education, even more when cooperative, since the acquisition of knowledge and enhancing skills now requires more actual approaches. The use of tablets, smartphones, social networks, etc. is more comprehensible and funny for young people compared to traditional media. The several roles allow everyone to enhance their own skills and are perfect for a full inclusion of Special Education Needs (SEN) students. We have already realized a first role playing computer game called GeoQuest [1] creating at the same time a Role Playing Engine [2] which can be easily applied to create new didactic games for the whole class. The outcome of the class experimentation were excellent, both for didactic and educational results obtained [3]. This game story is set under the Somma-Vesuvius volcano. The students go through a virtual environment, that gradually reveals itself: it is full of significant elements that can be traced back to a volcanic site, inserted in a specific geodynamic situation. Players can also discover where they are from the story of some historical and mythological figures they meet on their path. They can interact to solve several quests appearing during the game related to mineralogy, volcanology, geodynamics, history, myths.

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ECO innovative methodologies for the valorization of construction and urban waste into high grade TILES (ECOTILES, EU-LIFE project)

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The ECOTILES project aims at studying the possibility to produce high-grade cement-based tiles using glass and ceramic waste. The project, financed under the EU - LIFE ENVIRONMENT/WASTE program will contribute to the achievement of EU 2020 goals on waste and resource efficiency, reducing emissions, waste, impacts on human health and the environment. Specific objectives are to:

- Demonstrate an innovative methodology that integrates promising research results to produce a new generation of tiles made almost entirely (up to 70%) with recycled materials and with substantially lower environmental impacts compared to current products.
- Demonstrate the improved environmental performance in the production process of precast products, through the re-use and recycling of several streams of urban waste as well as lower energy consumption

LIFE ECOTILES project focus at:

- Design, implement, fine-tune and optimise a series of three versions of industrial precast-products (Terrazzo tiles) with up to 70% content of recycled materials, potentially improving mechanical and structural characteristics compared to current products made with virgin materials;
- Adapt and engineer a low-energy industrial process able to manufacture the recycled Terrazzo tiles on an industrial scale, consuming 20% less than traditional processes;
- Facilitate the recycling of up to 450 t/year of CDW and construction materials scrap and 3 000 t/year of glass waste, with a potential of around 1 000 times more in Europe if applied to a share of all pre-casted products;

More general expected results concern the a) building and maintaining a collection and valorisation network in the Marche region; b) increasing of the awareness of the improved eco-innovative solutions among the general public, policy-makers and in the European industry, focusing on the environmental and economic advantages and technical feasibility of innovations such as LIFE ECOTILES.

Why are soils different? A laboratory experience with the IBSE approach

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This didactic research project focus on investigating the characteristics of soil and interactions between different parameters influencing pedogenesis, like climate and the parent rock. The laboratory is part of a PhD project in the Geoscience education in UNICAM (UNICAMearth group). The purpose of this research is to produce didactic materials for students in the age range 11-14 years and for teachers without specific Geology background. The activity has been proposed using the IBSE (Inquire Based Science Education) approach which stimulates the formulation of questions and actions to solve problems and understand phenomena, contributing to the active learning, to promote collaboration among students and to enhance students' motivation, increasing knowledge and competences [1]. The soil is the topic of interest because it can represent a "fil rouge", allowing a strong interdisciplinary approach, giving the teachers the possibility to introduce Earth science topics (mineralogy, geology, geomorphology, climatology...) as well as other disciplines (biology, chemistry, technology, art..) The activity was tested on several classes with a control class. In the first part of the activity, students were divided into groups to investigate the IBSE-question: "why are soils different?", through the observation of totems describing stratigraphic columns, representing the formation of different soils with time, changing parent rock and climate conditions [2]. Paper-based information and guiding-questions are given to answer the principal question. The activity ends with a practical work and a discussion among the working groups. A pre-test and a post-test were given to the pupils to evaluate the learning outcomes. The results obtained from the experimentation show that the students were very involved in all the phases of the activity and interacting between each other, even those more reluctant to school. Using this activity they approached and deepened a topic which it is not usually taught in schools. The laboratory gives an opportunity to the teachers to attract the students attentions and to use the topic for interdisciplinary connections. Moreover it allows teachers to approach at a new educational science method.

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Dissemination of the geological subjects through the language of theatrical arts

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According to recent legislative and ministerial standards, teachers are required to change the way of "doing school" and to put "emphasis" on the needs in order to build a coherent and unified profile of cultural meanings through dialogue between the different disciplines. The National Guidelines regarding OSA (specific objectives of learning) according to the European directives based on the "knowledge society", recommend to improve interdisciplinary connections. The predominant linear path of disciplinary knowledge found in text books, enables a "schematic" mental state instead of leading to the "ability to connect", which could facilitate the development of complex thinking skills. This methodology resulted, over time, in a superficial knowledge that has led to the permanence of "misconception". In high school "laboratory practical experience [...] are promoted as a psychological mode, organizational, methodological, didactic, to have knowledge" (professional skills). The proposal of this research is to experience a laboratory of creative writing with a flipped classroom: the lectures and assignments are turned upside down. In the classroom there will be a debate on the personal studies. These are the questions that will be asked:

- Is the theatre "foreign" to science?
- Is it possible to promote scientific knowledge?
- Which form does provide a privileged access to science?
- Does this tool indicate the link between 'two cultures'?

We've analysed the precedent experiences and these are the results:

- Weaknesses: it's possible to put together theatre, science and school to get scientific education but it can also happen that one of these elements loses a part of its peculiarity.
- Strengths: lots of experiences in the school can be compared; theatre promotes a context of collective experience.

Our proposal was to produce a training module. We've realised a form for the scientific script with didactic value titled "The man and the mountain: the Mont Blanc".

The procedure provided for:

- The analysis of pedagogical needs;
- The presentation of the cases;
- The analysis of the misconceptions or prior knowledge;
- The selection of the scientific concepts we focused on;
- The application of the acquired knowledge.

The role of the teacher changed: he researches the material, writes the script with students, improves storytelling, assesses progress. Teachers from different disciplines must work together, creating the script with the students, who will be assessed during the creation of the scene and the dramatization, focusing on the show and the script.

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How Deep is "Deep Time"? A Teaching Experiment on the Learning of Geological Time

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Deep Time is considered a central concept within Earth sciences and other sciences with a historical dimension. While the understanding of conventional time has been investigated by cognitive research, the topic of Deep Time has been addressed by geology and evolution researchers. Since the pioneering studies of the 1980s, literature on the understanding of these concepts has grown significantly. However, most of these studies are descriptive or explanatory, with only a minority of interventional ones, none of which published in Italy at the time of the writing. Due to this gap in literature, an experiment on the learning of Deep Time e in a sample of Italian students was conducted. Our research hypotheses were: 1) can a short teaching activity improve the understanding of geological time concepts? 2) can a constructivist approach based on misconceptions be differently effective than a more traditional cognitivist approach? A randomized case-control trial (misconception-based vs. cognitivist teaching) was carried out through the following steps: a pre-test, an interactive lecture and a post-test. After about two months a third delayed test was administered to assess the long-term retaining of the learned concepts. The lecture addressed the history of Earth, with the addition - in the experimental group - of spatial models and questions aimed at eliciting cognitive conflict about Deep Time misconceptions. The assessment tool was built drawing from published research questionnaires, translating and adapting questions to the national school context. Questions addressed one or more of four basic concepts: succession, duration, dimensional scale and basic knowledge of stratigraphy principles. The sample consisted of 298 ninth grade students of liceo high schools located in Friuli Venezia Giulia, randomly allocated to the two groups of the trial. Significantly higher scores were recorded in both groups after the teaching activity, despite its short duration. Among the students who obtained equal or better scores in the post-test, the experimental group performed significantly better than the control group. The results suggest that even a short intervention on geological time may improve the understanding of the concepts related to this topic among 9th grade students. The higher scores in the delayed test in comparison with the post-test - without further teaching of the topic in the interval - raise some questions about a possible synergistic effect following the teaching of other subjects (history, maths) or the role of cognitive development during adolescence. We plan another enquiry with a longer teaching activity to further investigate the effect of the different approaches (misconception-based vs. cognitivist) tested in this study.

Fibrous Gypsum Veins as Diffuse Features and within Fault Zones: the Case Study of the Pisco Basin (Ica Desert, Southern Peru)

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New knowledge on patterns of fibrous gypsum veins, their genetic mechanisms, deformation style and weathering are provided by a field- and laboratory-based study carried out on the Neogene to Quaternary Pisco Basin sedimentary strata (porous sandstones, siltstones and diatomites) exposed in the Ica desert, southern Peru. Gypsum veins vary considerably in dimensions, attitudes and timing and can develop in layered and moderately fractured rocks also in the absence of evaporitic layers. Veins occur both as diffuse features, confined to certain stratigraphic levels, and localised within fault zones. Arrays formed by layer-bounded, mutually orthogonal sets of steeply-dipping gypsum veins are reported for the first time. Vein length, height and spacing depend on the thickness of the bed packages in which they are confined. Within fault zones, veins are partly a product of faulting but also inherited layer-bounded features along which faults are superimposed. Due to the different petrophysical properties with respect to the parent rocks and their susceptibility to textural and mineralogical modifications, water dissolution and rupture, gypsum veins may have a significant role in geofluid management. Depending on their patterns and grade of physical and chemical alteration, veins may influence geofluid circulation and storage, acting as barriers to flow and possibly also as conduits.

Fault-Controlled Dolomite Bodies as Geofluid Reservoirs and Paleotectonic Indicators: New Insights from Gargano Promontory Outcrops

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The Upper Jurassic to Lower Cretaceous platform-slope to basinal carbonate strata cropping out in the Gargano Promontory (southern Italy) are partly dolomitized. Although these dolomite bodies were discovered and mapped a half century ago, they have so far not been comprehensively characterized. This study relies on fieldwork and laboratory analyses (petrographic, geochemical and petrophysical), and aims at characterizing the distribution of the dolomite bodies within the carbonate succession, their dimensions, geometries, textural variability, chemical stability, age, porosity, genetic mechanisms and relation with tectonics. The investigated dolomite bodies range from meters to kilometers in size, are fault- and fracture-related, and likely formed during the Early Cretaceous at $<$ 500 m burial depths. The proposed dolomitization model relies on mobilization of low-temperature ($<$ 50°C), modified marine formation water that circulated along faults and fractures. During the Cenozoic exhumation of the Gargano carbonate succession, dolomite bodies were partly dedolomitized by meteoric waters, especially in their peripheral zones. Distribution and geometries of dolomite bodies provide new evidence for Early Cretaceous brittle tectonics in southern Italy, as NW-SE to E-W striking paleo-faults, from meters to 10's of kilometers in size, and likely with normal to right-lateral strike-slip kinematics. As dolomitization increases by up to 7% the matrix porosity and, hence, can improve the geofluid storage capacity of tight, platform-slope to basinal limestones, the results have a great significance for characterization of hydrocarbon reservoirs, for instance those of the Adriatic offshore area, many of which are hosted in similar dolomitized carbonate successions.

Faulting of a turbidite sandstone-siltstone successions: the case study of the Macigno Formation, Tuscany, Italy

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Faults in siliciclastic rocks are characterized by a great variability of fault zone architecture and relative permeability properties. This is because siliciclastic rocks (i.e turbidites) are often represented by alternating beds of various thickness and grain size forming succession of contrasting mechanical properties. For example, the presence of sandstone and clay-rich layers is responsible for the simultaneous occurrence of brittle and ductile deformation, known as "clay smear structures". Moreover, numerous studies have identified grain size as one of the main influencing factors for fault nucleation processes and fracture intensity in the damage zone [1,2].

In this work, we present the results of field and laboratory analyses performed on the Macigno Formation cropping out along the coast in western Tuscany. Here, the Macigno Formation is represented by Late Oligocene foredeep siliciclastic succession dominated by turbidite sandstones with minor siltstones, mudstones, marls and shales. The thickness of the sandstone and siltstone beds varies significantly from tens of centimetres up to 4 metres and from several centimetres up to tens of centimetres, respectively. Thin section and 3D analyses, performed by X-ray Synchrotron microtomography, allowed us to characterize grains, especially their geometrical and morphological properties (e.g. size, shape, specific surface area). We documented how both the grain size and the mechanical properties of the alternating beds strongly control the fault zone architecture, in particular in terms of damage zone thickness and fracture frequency. The fault rock types (i.e. breccia vs. gauge) are strictly related to the amount of displacement as well as to the grain size and the cementation of the sandstone. Furthermore, the development of clay smear structures is enhanced by the presence of interbedded thin clay-rich layers.

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A water solubility study in pantelleritic glasses to 250 MPa

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The solubility of H_2O in pantelleritic glasses has been investigated experimentally in the range of 800-900°C ad pressures of 50, 100, 150 and 250 MPa. The water concentration has been determined by FTIR and Raman spectroscopy. Using a synthetic glass analog of pantelleritic magma of Kenya Rift Valley (Ebu-1 in [1]) as starting composition, the molar Na/(Na+K) ratio was varied from 0 (Ebu-C) to 0.74 (Ebu-B) and 1 (Ebu-N) at constant total alkali content. The alkali effect has important implications for the chemical and physical properties of rhyolitic melts [2] and such dependence for pantellerites is still poorly constrained. The compositional dependence of water solubility as a function of Na/(Na+K) was investigated at 840°C in the pressure interval 50-150 MPa and results suggest that Na favors H_2O solubility on equimolar basis. The effect of pressure (P) on H_2O solubility can be reported as nearly linear positive correlation between P and H_2O solubility in the P-T ranges investigated, between 50 and 150 MPa at 840°C and between 50 and 250 MPa at 800°C. The temperature influence has been studied in a minor range (800-900°C) and water solubility ranged from 4.80 ± 0.10 wt % to 7 ± 0.13 wt % with decreasing temperature at 150 MPa through temperature independence at approximately 50 MPa. These data will be useful in order to implement existing predictive models of solubility over a wider range of silicate melt compositions and to better understand magma degassing processes.

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2D XANES mapping of heterogeneous samples: an application to natural volcanic glasses

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X-ray Absorption Near Edge Structure (XANES) imaging with synchrotron radiation is a powerful tool for the characterization of heterogeneous samples such as rocks or cultural heritage artefacts. The spatial distribution of the different elements (elemental maps) within the sample can be monitored by collecting a single XRF map at fixed energy above the edges of the elements of interest. Beyond this, and thanks to the tunable energy provided by the synchrotron source, XRF maps can be collected at characteristic energy values around the absorption edge of a specific element (e.g. pre-edge peaks, inflection point, white line) to enhance the contribution from a particular valence state or site symmetry of the absorber. Therefore changes of oxidation state and coordination geometry of elements within the sampled area in heterogeneous samples can be also monitored. Because of the fluorescence detection, even trace elements with concentration in the ppm range can be studied. Here we report XANES imaging experiments performed at the Italian beamline (LISA-BM08) of the European Synchrotron Radiation Facility on thin sections of natural volcanic glasses from Pantelleria Island (Italy). By using an x-ray spot of 200μmx200μm, we collected x-ray fluorescence maps at different energies across the Fe K-edge. From the analysis of XRF maps collected above the absorption edge and on selected features of the XANES such as the edge and pre-edge peaks, we obtained qualitative information on the spatial distribution of iron in the sample as well as on variations of the Fe oxidation state and local symmetry within the sampled area. After the two-dimensional elemental and chemical mapping, full XANES spectra were collected in selected points in order to extract quantitative information on the Fe oxidation state and coordination from the pre-edge peak fitting. The experiments here reported find application for the characterization of cm-sized zones of heterogeneous samples for which the extreme spatial resolution achieved with micro/nano beams is not needed.

From Fracture Analysis to Flow Simulations of an Outcropping Hydrocarbon Reservoir (The Roman Valley Quarry, Majella Mountain)

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The Roman Valley Quarry located at the northern termination of the Majella anticline in central Italy contains an excellent exposure of bitumen-bearing faulted carbonates, and there-fore provides the opportunity to assess the role of stratigraphic and structural heterogeneities on subsurface flow. The vertical walls of this quarry expose in 3D the inner structure of two oblique-slip normal faults oriented WNW-ESE (called the SW and NE Faults). These faults crosscut the Oligo-Miocene Bolognano Formation, which is a medium- to high-porosity lime-stone (Cilona et al., 2014)2. The SW Fault has a seismically detectable throw of 40 m, and consists of a continuous main slip surface, with fault rocks that vary along strike from clast- and cement-supported cataclastic rock to un-cemented breccia. This fault behaves as both a conduit and barrier for fluid flow. Conversely, the NE Fault, which has a sub-seismic throw of 8 m, consists of a fractured zone where several smaller slip panels interact, forming a distributed conduit permeability structure (Agosta et al., 2010)1. Laboratory measurements and detailed Discrete Fracture Network (DFN) models are inte-grated to quantify matrix and fracture contribution to porosity and permeability within each of the lithofacies cropping out in the study area. DFN models were constrained by spatial and dimensional properties of fractures obtained by scanline surveys. These models were used to calculate fracture permeability and porosity based on the Oda upscaling method. Finally, the obtained hydraulic properties were used to build an outcrop-scale static model of both the matrix and the fractures. This model is useful to build flow simulations to test fluid pathways for various flow scenarios showing the role played by the stratigraphic and structural heterogeneities.

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3D Pore-Network Analysis and Fluid Flow Simulation in Deformation Bands Hosted in Carbonate Grainstones.

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In porous rocks strain is commonly localized in narrow Deformation Bands (DBs), where the petrophysical properties are significantly modified with respect the pristine rock [1, 2]. DBs could have an important effect on production and development of porous reservoirs representing baffles zones or, in some cases, contribute to reservoir compartmentalization [3]. Taking in consideration that the decrease of permeability within DBs is related to changes in the porous network properties (porosity, connectivity) and the pores morphology (size distribution, specific surface area), an accurate porous network characterization is useful for understanding both the effect of deformation banding on the porous network and their influence upon fluid flow through the deformed rocks. In this work, a 3D characterization of the microstructure and texture of DBs hosted in porous carbonate grainstones was obtained at the Elettra laboratory (Trieste, Italy) by using two different techniques: phase-contrast synchrotron radiation computed microtomography (micro-CT) and microfocus X-ray micro-CT. These techniques are suitable for addressing quantitative analysis of the porous network and implementing computer fluid dynamics experiments in porous rocks. Evaluated samples correspond to grainstones highly affected by DBs exposed in San Vito Lo Capo peninsula (Sicily, Italy), Favignana Island (Sicily, Italy) and Majella Mountain (Abruzzo, Italy). The evaluated properties were porosity, connectivity and specific surface area. Permeability was estimated by using Lattice-Boltzmann simulation; results are validated by comparing with in situ permeability measurements.

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Mathematics

How to solve a passive safety problem through a multidisciplinary approach

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The term "passive safety" refers to all design measures taken to protect the driver and the passengers from injury. Besides the seat belt system, the most important passive safety features in a car include the airbags, the 'deformation-resistant" occupant cell and the front and rear deformation zones. The last ones provide a substantial amount of protection by dissipating the impact energy through a progressive crushing; more regular and smooth is the deceleration versus time signal that is recorded during a collision, less risk of injury can be estimated. The research work, done in collaboration with the spin-off Limix and the group of Prof. Belingardi of Politecnico di Torino, refers to the resolution of passive safety problems from a mathematical, numerical and experimental point of view; in particular it studies the analytical equations governing the energy absorption of specific impact attenuators, varying geometry and material used, and the structural optimization in order to pass specific homologation tests imposed by European legislation. The models validation is possible thanks to experimental investigation able to capture the real phenomenon; despite the complexity of the problem the proposed analytical and numerical analyses reproduce the results with a good level of accuracy.

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Refrigerator ladies

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In 1942, when computers were human and women were underestimated, a group of female mathematicians helped win a war and usher in the modern computer age. The ENIAC, the first electronic, digital, general purpose computer, was part of a ministry of the US defense secret project during World War II. The six young women mathematicians developed all its software while programming languages, or even manuals and operating systems, were not available; without knowing its architecture, they became experts of the new computer and they planned with complicated calculations successful ballistic trajectories, founding the modern programming. In 1946, with the execution of the first program, the project became public and had enormous repercussions in the press, but the ENIAC's success was attributed only to the engineers who built it. The history of its programmer girls was lost. For a long time the young women photographed together with the huge machine full of plugs and wires were exchanged for models posing next to an electrical appliance! A programmer at Harvard, in the eighties, rebuilt the story, interviewing some of them directly and highlighting the incredible work they were able to carry on. In our paper we tell the story of the ENIAC women, highlighting first the mathematics underlying the ballistic problems emerged during World War II, that the Eniac and its human calculators were called upon to solve, and then describing the ENIAC's architecture and the issues raised in its programming.

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Unicam Science Outreach: F.A.R. as communication can

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According to the European Charter for Researchers " researchers should ensure ... that the results of their research are disseminated and exploited, e.g. communicated, transferred into other research settings or, if appropriate, commercialised ..."

Therefore, it's part of the researchers' mission to raise the general public awareness with respect to science. This need is further emphasized by a survey of Eurobarometer 2010: society is strongly interested in science but, at the same time, is often scared by the risks connected with new technologies. Moreover, irrational attitudes towards science are prompted by a broad scientific illiteracy. The result is a remarkable distance between the community of scientists and the society at large. How to fill this gap? Science communication requires a specific training, which is not part of the average researchers education. Unicam Science Outreach is a project leaded by an interdisciplinary team of researchers with all the skills and competences for a correct and sound scientific communication. Its aim is to design and develop effective communication strategies, targeted to the background and needs of the audience: from policy makers to potential industrial partners, from youth and school teachers to the general public. We describe the activities undertaken so far in the framework of the project, and we outline those planned over the next months.

Optimal Output Regulation for Weakly Dual Redundant Plants

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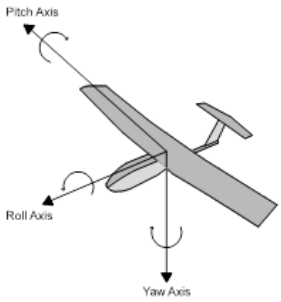
Control allocation is an important problem in several applications where multiple actuators are present, and their number is larger than the number of outputs to be controlled; several such examples arise in the context of aircraft control, marine vehicles, double actuator positioning in hard disks and several others [1], [2]. In our research, we study the dual problem of output redundancy, which is the opposite setup where a redundant number of outputs is present. Such dual redundancy is a typical characteristic of under-actuated systems. Classical examples of under-actuated mechanical systems can be found in the framework of autonomous robots, such as underwater vehicles and aerial vehicles (see figure). The output redundancy problem becomes particularly interesting and prioritary in the event of failures during critical operations, such as dynamic positioning for marine vessels or flight in harsh environments for unmanned aircrafts [3]. The aim of our research is to investigate how to use dual redundancy in a clever way, and we will focus specifically on the regulation problem. When a system is under-actuated, only a subset of the outputs can be arbitrarily controlled, and the remaining ones are constrained. 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.



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Body cognition and math education for pre-school children

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In every type of dance, from the traditional and the classical ones up to the modern, there are many mathematical concepts. Some of them are unconsciously used, both to find harmony of human bodies in the space, and for the logic. In contemporary dance techniques some choreographer noticed the strong presence of math and decided to taking inspiration from them. With this project we explore the connections between mathematics and dance, understood as a movement of the body itself. The Dance show “Intrecci” is presented in a video (15’ long): it shows the presence of topological and geometrical elements not only for help public to see some abstract object, but also to make the audience aware of how maths is presented in everyday life. Words, scenography and images are essential and helpful for the audience to focus the attention on the dancers’ lines and bodies. The music has been chosen with attention: "Knee 5" from "Einstein on the beach" and "Metamorphosis 1" were composed by Philip Glass; their melody and sonority allow to exalt choreographs elements. The "Body Percussion Song" is a clapping music song, that is music composed only whit body, voice and percussion; it was chosen for its energy. The performances that can be seen in this video can be used for every level school project. In fact, we experimented it in a kindergarten (I.S. Serravalle (MC)). The idea is to use the human body and the space that surrounds it in order to introduce important and (in this case) basic concepts of Geometry and, in general, Mathematics.

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Homotopic intersection form of a surface and positivity in the mapping class group.

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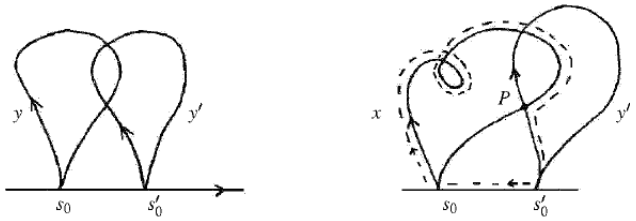
Let S be a compact, connected, oriented surface of genus g, with b boundary components ($b \geq 1$), δS. Fix a base point $s_0 \in \delta S$ in one of the boundary components, we set $\Gamma = \pi_1(S, s_0)$ the fundamental group. In [2] (as in [4]), Perron exhibits that there exits a map $\omega : \Gamma \times \Gamma \to \mathbb{Z}[\Gamma]$,

$$\omega(x, y) = \sum_{P \in x \cap y} e_P g_P \in \mathbb{Z}[\Gamma],$$



called *homotopic intersection form* such that:

1. $\omega(y, x) = -\overline{\omega(x, y)} + (y - 1)(x^{-1} - 1)$,
2. $\omega(xy, z) = \omega(x, z) + x\omega(y, z)$,
3. $\omega(x, yz) = \omega(x, y) + \omega(x, z)y^{-1}$,

From [5] we know that, taking a diffeomorphism $f : S \to S$ fixing the boundary pointwise, f is right-veering if and only if $\omega_1(f * \alpha, \alpha)$ id odd for any $\alpha \in \pi(S, s_0)$. The concept of right-veering is important in the field of Low dimension Contact Topology: in [6] we understand the relationship to tight contact structures and open book decompositions.

At this stage we are working on the idea of define a kind of gradualness of right-veeringness, using other ω_δ with $\delta \in \pi(S, s_0)$, $\delta \neq 1$, and trying to turn simple diffeomorphisms into right-veering, after doing n-positive Dehn twists.

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Factorization Machines and Recommender Systems

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Recommender Systems (RS) [1] are a specific type of information filtering techniques which attempts to present to the user, in an innovative and personalized way, the items she is interested in. "Item" is a general term used to denote what the system recommends to the user and, depending on the domain of interest, can be a movie, a song, a research article, a person who she may know in a social network and so forth. The target can be reached through two different ways: the collaborative approach [1] exploits information about the past behaviour and opinions of an existing users community to predict which item the current user will be more interested in, while the content-based approach [1] relies on additional information about user's preferences and, above all, on the items content, that is the description of items characteristics. Both approaches have strengths and weaknesses, but to reduce the latter, they are often combined in hybrid methods.
Factorization machines [3] are a new model class that combines the advantages of Support Vector Machines (SVMs) [2] with factorization models and have been proved to behave successfully in parameters estimation even in the sparse settings where SVMs alone would fail. Factorization machines are able to capture the interaction between user's and items under a hybrid scenario: they let to specify both users and items features. We propose to exploit the item "content" retrieved from the Linked Open Data cloud [4] and in particular from the structured version of Wikipedia, i.e. `DBpedia`, to improve the state of the art results of hybrid systems in terms of accuracy and precision.

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Physics

Mechanical EPR entanglement and optomechanical cooling with a finite-bandwidth squeezed reservoir

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We propose schemes for the generation of non-classical states of a nano-mechanical resonator beyond the resolved sideband regime with a finite-bandwidth squeezed reservoir. In a first scheme, we describe a scheme for the generation of mechanical EPR entanglement employing the radiation pressure force of the squeezed light produced by a degenerate optical parametric oscillator, which acts as a reservoir of quantum correlations (squeezed reservoir) [1]. In a second scheme [2], we analyze the performance of optomecahnical cooling in the presence of a squeezed reservoir. More in detail we demonstrate that, when certain phase matching condition between pump laser phase and squeezing phase are met, the squeezed light can serve to suppress the residual mechanical diffusion due to blue sideband transition (back-action noise) and hence to enhance the cooling efficiency.

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SEI formation and evolution in graphite and ZFO-C electrodes probed by X-ray absorption spectroscopy

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Rechargeable lithium-ion cells battery are widely used today for commercial applications due to their high energy density, and good cyclablity. Starting from the first full cycle of the cell a layer of decomposed electrolyte, called SEI (solid electrolyte interphase), forms on the electrodes surface; this leads to alterations of efficiency, durability and to an irreversible capacity loss. Understanding the complex surface chemistry of the electrodes is crucial for enhancing the long-term variability of those cells [1,2]. Graphite is widely used as commercial carbon insertion host due to its relatively high capacity (372 mAh/g), safety and low cost. More recently, zinc ferrite ($ZnFe_2O_4$) encapsulated in a carbonaceous matrix (ZFO-C) has been proposed as mixed alloying-conversion anode material showing an higher charge/discharge capacity and cycling efficiency mostly related to the formation of a stable and efficient SEI layer [3]. In this work, performed within an European FP7 project (SIRBATT) collaboration effort, we present a study of the SEI at selected anode capacities using the technique of X-ray absorption spectroscopy (XAS). Arsenic atoms, present in the electrolyte as Li salts ($LiAsF_6$), are used as local probe for As K-edge XAS for monitoring the SEI evolution on the electrodes. Analysis of X-ray Absorption Near-Edge spectra has been performed to measure the quantity of As in its different valence states, then, Extended X-ray Absorption Fine Structure refinement [4] has been used for the detailed characterization of the local structure around As atoms within the SEI. Those experiments gave unique results about the SEI evolution [5]: as the estimated thickness, weight of different As oxidation states, average As - F distances and coordination numbers.

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Optical simulation and modelling for LED lighting components

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The market share of lighting products based on LED (Light Emitting Diode) source is rapidly growing, and it is projected to become the dominant technology before the end of the decade. The sustained research effort over recent years have resulted in a steady increase in performance, compared to traditional light sources. In the context of the Eureka project, at the Innovation Lab of the iGuzzini illuminazione company in Recanati, my research activity focuses on the development of optical components optimized for LED lighting. The human eye perceives the visible part of the electromagnetic spectrum, and the usual radiometric SI quantities (Watt for power) are scaled to photometric quantities (lumen for flux), according to our sensitivity to different wavelengths. Optical design is the technique of modelling reflective and refractive components able to manipulate light coming from one or more sources. The ray-tracing software allows the designer to simulate intensity distribution and efficiency, as well as the CIE color illuminance of a target. By means of this powerful tool, the presented work shows the wide variety of optical configurations I designed, according to the best photometric curve needed by each application. Exploiting the Total Internal Reflection (TIR) phenomenon, transparent plastic lenses can be used to collimate light from LEDs for spot applications both for wide external areas (architectural lighting) and smaller internal environments (museums and shops). Also, the designed diffusing screens may be added to obtain flood and wide flood distributions. In all cases, a very reliable accordance between simulated and measured outputs has been found. On the other hand, street lighting represents probably the hardest context for optical design, because of the many distribution parameters to be obeyed. Thereby, I modelled an aluminum reflector and a plastic PMMA lens for different projects. The result is that both of them are able to illuminate the street: both simulated and measured photometric curves satisfied luminance guidelines, even with quite different shapes. Furthermore, since LEDs are rapidly improving, one has to consider that emission and dimension of the source may change.

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A learning progression on basic astronomical phenomena

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Research in science education highlighted the role of a learning progression approach to describe and interpret how students develop their understanding of a given concept from naive ideas (lower anchor), to the scientifically correct idea (upper anchor) (Duncan & Hmelo-Silver, 2009; Duschl, Schweingruber & Shouse, 2007; Stevens, Delgado & Krajcik, 2010). Designing and validating a learning progression is a research-based process (Neumann, Viering, Boone & Fischer, 2013): first, an initial learning progression is hypothesized from literature and syllabus analysis; then, a measurement instrument is designed to inquiry into students' ideas and assess alignment between the hypothesised learning progression and the actual students' achievements. If the alignment is poor, the measurement instrument and the initial learning progression need to be revised. In this research project, we developed a learning progression about basic astronomical phenomena - change of seasons, lunar and solar eclipses and Moon phases. We first hypothesised an hypothetical learning progression, then we designed a mixed true/false multiple-choice questionnaire as measurement instrument, and finally compared the learning progression with secondary school students (14-18 years old) achievements in the questionnaire. Students' answers were analysed using Rasch analysis. Results allowed us to revise the initial learning progression (Testa, Galano, Leccia & Puddu, 2015). The revised version of the learning progression was then tested with prospective teachers, showing a satisfying alignment. As further step, we will investigate the alignment of the revised learning progression with middle school students' achievements using an adapted version of the original measurement instrument.

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Pairing and Condensation in Two-Dimensional Bose-Fermi Mixtures

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A unique opportunity to explore pairing phenomena is provided by ultracold gases of particles. In this context, Bose-Fermi mixtures have been object of a large theoretical and experimental investigation over the last fifteen years. By exploiting Fano-Feshbach resonances[1], the formation of ultracold heteronuclear molecules has been achieved in such systems[2]. We here present a non-perturbative theory that is able to describe a two-dimensional Bose-Fermi mixture across a broad interspecies Fano-Feshbach resonance, extending our previous work for a three-dimensional system[3]. The reduced dimensionality of the system here at issue provides the possibility to tune independently the boson-boson and the boson-fermion interactions via a Fano-Feshbach resonance and a confinement-induced resonance[4]: this could be the key point to have a mechanically stable Bose-Fermi mixture for a wide range of boson-fermion couplings which would favour the experimental investigation. Indeed, a sufficiently large value of the boson-boson repulsion is required to ensure the mechanical stability of the mixture[5]. We present numerical results for chemical potentials and condensate fraction of bosons, providing further a comparison with perturbative results derived for weak boson-fermion couplings.

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X-ray absorption spectroscopy: new insights on the three-dimensional liquid structure

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The local structure of liquid metals and binary metal alloys may differ significantly from that of the corresponding crystalline systems, possibly containing icosahedral local ordering, forbidden in periodic structures. The application of Reverse Monte Carlo (RMC) for combined refinements of XAS and diffraction data allowed us to obtain in selected liquid metals an ensemble of realistic three-dimensional models of the liquid structure, compared also with the results of molecular dynamics simulations. In previous works, signatures of short-range fivefold ordering have been investigated by x-ray absorption spectroscopy (XAS) experiments in elemental liquids including for example, liquid and undercooled copper and nickel for which estimates of the fraction of nearly-icosahedral configurations were obtained [1,2]. We have recently improved our RMC-XAS method [3], extending its application to multi-atomic substances, performing also several XAS experiments in liquid metals at high temperatures. In this work, we report RMC refinements of accurate XAS data of several molten elemental metals and binary alloys showing that an accurate reconstruction of the three-dimensional local structure is feasible. The results of our work include estimates of the fraction of atoms having local icosahedral symmetry, in elemental metals like Cu, Ni, Cd. Moreover, a detailed analysis of local coordination and geometry in molten alloys such as Cu-Sn and In-Sn is presented.

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Microfabrication of high-stress SiN membranes with arbitrary shape for optomechanical applications

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Optomechanical setups span a vast range of sizes and masses, as do their applications and aims - from testing the foundations of the quantum theory to precision sensing and detecting gravitational waves[1–5]. More generally speaking, these experiments are performed not only in the optical, but also in the microwave domain. The two meet in efforts to develop an optical-to-microwave transducer, which would, in turn, be of use in quantum computing. In view of the integration of membrane resonators with more complex microelectromechanical systems (MEMS)[6], we developed a general fabrication procedure for circular shape SiNx membranes using deep reactive ion etching (DRIE)[7]. The membranes were used as resonators in a Michelson interferometer and a Fabry-Pérot cavity to study their properties. Albeit the fabrication procedure has yet to be optimized, both mechanical quality factors and optical roughness are comparable to those of commercially available membranes, while the optical absorption is almost an order of magnitude lower. Finally, we present our ongoing work in trying to achieve three-mode coupling in a membrane-in-the-middle optomechanical setup, which would also encompass ground state cooling of the mechanical mode and squeezing in the output light.

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Generation and detection of large and robust entanglement between two different mechanical resonators in cavity optomechanics

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We investigate a general scheme for generating, either dynamically or in the steady state, continuous variable entanglement between two mechanical resonators with different frequencies. We employ an optomechanical system in which a single optical cavity mode driven by a suitably chosen two-tone field is coupled to the two resonators. Significantly large mechanical entanglement can be achieved, which is extremely robust with respect to temperature.

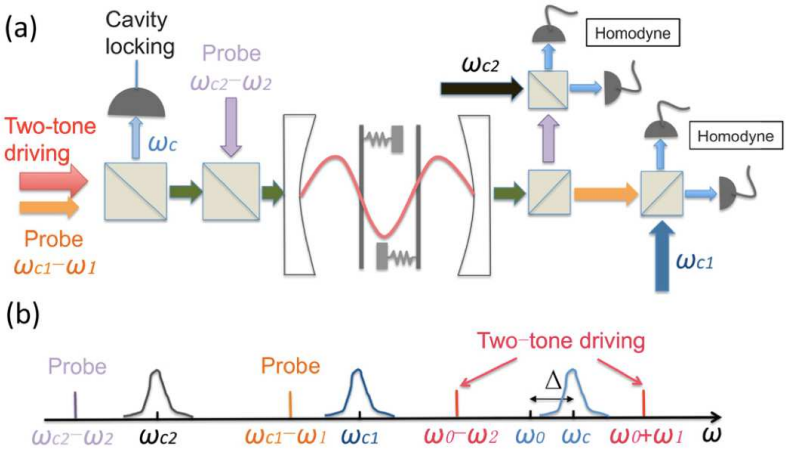

Figure 1. Sketch of the proposed entanglement generation and detection scheme (a), and of the various pump and probe laser frequencies (b). The cavity mode is bichromatically driven at the two frequencies $\omega_0 + \omega_1$ and $\omega_0 - \omega_2$. Large and robust entanglement of the two mechanical resonators can be generated either dynamically or in the steady state. Two weak probe fields with detuning $\Delta_j^p = \omega_{cj} - \omega_j^p = \omega_j$, $j = 1, 2$, are then sent into the cavity. By homodyning the probe mode outputs, the mechanical quadratures (x_j, p_j) are therefore measured, which allows one to construct the correlation matrix of the quadratures from which entanglement can be derived in a straightforward way.

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Controlling electroosmotic flows by polymer coatings: A joint experimental-theoretical investigation

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We analyze the electroosmotic flow (EOF) of an electrolytic solution in a polymer coated capillary electrophoresis tube. The polymeric density, charge, thickness, and the capillary tube charge vary as a function of pH and produce a non-trivial modulation of the EOF, including a flow reversal at acid pH conditions. By means of a theoretical argument and numerical simulations, we recover the experimental curve for the EOF, providing a firm approach for predictive analysis of electroosmosis under different polymeric coating conditions. A proposed application of the approach is to determine the near-wall charge of the coating to be used for further quantitative analysis of the electroosmotic flow and mobility .

Our work is particularly useful because it asserts that the simple one-dimensional description of the system, under the assumption of a linear Poisson-Boltzmann solution for the EDL and by assimilating the coating region to a porous medium, is accurate enough for quantitative analysis.

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Multidimensional Stationary Probability Distribution for Interacting Active Particles

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We derive the stationary probability distribution for a non-equilibrium system composed by an arbitrary number of degrees of freedom that are subject to Gaussian colored noise and a conservative potential. This is based on a multidimensional version of the Unified Colored Noise Approximation. By comparing theory with numerical simulations we demonstrate that the theoretical probability density quantitatively describes the accumulation of active particles around repulsive obstacles. In particular, for two particles with repulsive interactions, the probability of close contact decreases when one of the two particle is pinned. Moreover, in the case of isotropic confining potentials, the radial density profile shows a non trivial scaling with radius. Finally we show that the theory well approximates the "pressure" generated by the active particles allowing to derive an equation of state for a system of non-interacting colored noise-driven particles.

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Velocity distribution in active particles systems

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We derive an analytic expression for the distribution of velocities of multiple interacting active particles which we test by numerical simulations. In clear contrast with equilibrium we find that the velocities are coupled to positions. Our model shows that, even for two particles only, the individual velocities display a variance depending on the interparticle separation and the emergence of correlations between the velocities of the particles. When considering systems composed of many particles we find an analytic expression connecting the overall velocity variance to density, at the mean-field level, and to the pair distribution function valid in the limit of small noise correlation times. Finally we discuss the intriguing analogies and main differences between our effective free energy functional and the theoretical scenario proposed so far for phase-separating active particles.

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Towards a statistical mechanical theory of active fluids

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We present a stochastic description of a model of N mutually repelling active spheres in the presence of external fields and characterize its steady state behavior. To reproduce the effects of the experimentally observed persistence of the trajectories of the active particles we consider a Gaussian forcing having a non vanishing correlation time, whose finiteness is a measure of the activity of the system. With these ingredients we show that it is possible to develop a statistical mechanical approach similar to the one employed in the study of equilibrium liquids and to obtain the explicit form of the many-particle distribution function by means of the multidimensional unified colored noise approximation. Such a distribution plays a role analogous to the Gibbs distribution in equilibrium statistical mechanics and provides a complete information about the microscopic state of the system. pair correlations and the pressure of active fluids. In the low density regime we obtain the effective pair potential.

Effective potential method for active particles

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We investigate the steady state properties of an active fluid modeled as an assembly of soft repulsive spheres subjected to Gaussian colored noise. Such a noise captures one of the salient aspects of active particles, namely the persistence of their motion and determines a variety of novel features with respect to familiar passive fluids. We show that within the so-called multidimensional unified colored noise approximation, recently introduced in the field of active matter, the model can be treated by methods similar to those employed in the study of standard molecular fluids. The system shows a tendency of the particles to aggregate even in the presence of purely repulsive forces because the combined action of colored noise and interactions enhances the the effective friction between nearby particles. We also discuss whether an effective two-body potential approach, which would allow to employ methods similar to those of density functional theory, is appropriate. The limits of such an approximation are discussed.

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Structure and chemical composition reversibility during Li-ion rocking chair battery operation based on ZFO anodes

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Structure and composition changes of ZFO-C (carbon covered $ZnFe_2O_4$) nanoparticles [1] used in anodes during Li+ batteries charge and discharge cycles was monitored at the atomic level as a function of time by using XAS [2], a chemical sensitive and short range probe, and by selectively tuning the detection depth by collecting electrons, total and partial yield, and photon fluorescence yield. ZFO ($ZnFe_2O_4$) spinel partially inverts [1] after Li insertion in octahedral sites and concomitant migration of Zn from tetrahedral sites. This mechanism is competitive with the conversion alloying mechanism of LiO_2, LiZn and separation of metallic Fe. The reversibility of the present transformation is difficult to be tracked by conventional techniques as the disorder dominates and the diffraction techniques fail in following the microscopic phases during the charging and discharging cycle. X-ray absorption experiments have been conceived and realized to study the modification of the signals related to the structure during the lithiation process. To this aim a full multiple scattering calculation was employed, with assistance of full potential to best treat the open structures by using a virtual bcc network of empty spheres. This method will be used for k-shells while L2,3 edges will be studied by means of the empirical program (CTM4XAS) [3]. The nanostructrues of the anode material, consisting of 30-50 nm size covered ZFO particles covered by C, interact with battery environment made by binder (carboxymethylcellulose) , solid electrolyte ($LiPF_6$) and solvent (mixture of ethylene and dimethyl carbonate). XAS allows to grasp the inner mechanisms of the interface formation and cycling mechanism at the basis of the high capacitance material. In particular the role of the surface and of a partially reversible interface increasing the Li storage limit is under study by the present methods.

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Mechanically-Induced Transparency in a hybrid electromechanical system

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We study an electromechanical hybrid system consisting of a radiofrequency (rf) resonator coupled to a mechanical resonator. The oscillation of the mechanical resonator can alter the capacitance of the radiofrequency resonator leading to the modulation of transmitted signal. The coupling between the two resonators manifests itself by an effect called Mechanically-Induced Transparency (MIT), which is an interference effect like the well known phenomenon Electromagnetically- Induced Transparency (EIT). In our study the rf resonator is an LC with variable resonance frequency between 100 kHz -1MHz. The quality factor of the resonator is around 130. The hybrid system is obtained by coupling the LC resonator to a metalized high stress, 1×1 mm^2, 50 nm thick, stoichiometric Silicon Nitride Membrane. We drove the electronic resonator with an rf signal and observed an MIT transparency window in the transmitted signal. We measured the coupling rate in two independent ways using the electronic signal as well as the reflected optical signal.

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Anisotropy effects in cosmological Entanglement

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Most existing cosmological entanglement studies are focused on the isotropic Robertson Walker (RW) space-times. However for a more realistic cosmological model that represents the Universe, it is necessary to take anisotropy into account. Here we study the influence of the anisotropy on the entanglement generated by dynamical space-times. Since the isotropic space-time is viewed as a background medium, and the anionotropy is incorporated as perturbation, we decomposed the entanglement entropy into the isotropic and anisotropic contributions. Our analysis is illustrated for two cosmological models with weakly and conformal coupling. We also study the possibility of using the entanglement to infer about universe features.

Superconducting regime in ultra thin Niobium nanofilms

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We have investigated the metallic state and superconducting properties of high quality Niobium nano-films as a function of their thickness, in order to study the transport properties and the quantum size oscillations of the superconducting critical temperature, Tc, in the ultranarrow regime. We have also characterized the interaction between the substrate and the Niobium nano-films which is responsible for an overall trend of suppression of Tc due to an inverse proximity effect. Layers with several thicknesses, varying from about 8 nm to 80 nm, have been deposited by sputtering on the oxidized surface of silicon wafers and then characterized by measurements of the temperature dependent resistivity (see figure below) and current-voltage characteristics. We found that Tc, as an overall trend, lowers for decreasing thickness while the width of the Tc resulted at least one order of magnitude lower than data reported in the literature. These very narrow widths of the superconducting phase transition indicate remarkable high structural quality of our Nb nanofilms, which is a key prerequisite for further nanostructuring pointing toward Nb nanostripes. On top of the overall decrease we found a small oscillatory behavior of Tc which we attribute to the quantum size effects and the shape resonances due to the strong confinement of the nanometer thick films along the transversal direction. This demonstrates a sizable interplay between quantum size effects and (anti)proximity effects in the superconducting phase of the nanofilms.

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Geometrically induced DOS effect on electronic transport properties of Si nanowires

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Semiconducting nanowires (NW) have recently been extensively studied and developed for applications in nanoelectronics, optoelectronics, solar cells and sensors using carriers con- finement[1,2]. The Si and Ge NWs, in particular, can be promising candidates for one-dimensional superconductor-semiconductor hybrid systems[3,4]. However, their electronic transport properties are strongly dependent on their surface and core structure. Hence, a detailed study on their possible effects on these properties are necessary prior to utilization of such hybrid systems. Here, we have studied electronic transport properties as a function of the temperature of Si NWs with two distinct structures. One with embedded Si quantum dots and the other with a percolative crystalline path. We show that the predesigned structure of the wires results in a prominent single distinct conduction mechanism such as tunneling in the former case and variable range hopping in the latter case[5]. We demonstrate that measured transport properties are the result of the geometry of the systems, with a large internal surface having a significantly high density of states. These results improve the understanding of the basis of the different electronic transport mechanisms in silicon nanowires and can lead to advanced hybrid systems design with a high controllability and precision.

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Nanostructure-Based Fluorescent Biosensors

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We have investigated a fluorescent biosensor based on graphene oxide (GO) for the measurement of interaction between a fluorophore FAM (Carboxyfluorescein)-labeled single-stranded DNA with its complementary single-stranded DNA oligonucleotide (target). The graphene oxide adsorbs the FAM-labeled single stranded DNA (probe) and quenches its fluorescence. Upon addition of the complementary single stranded DNA oligonucleotide, the probe hybridizes to its target [1] thus producing a double- stranded DNA, which detaches from the GO. The release of the double helix leads to the recovery of dye fluorescence that can be monitored by fluorimetric techniques. Pristine GO [2,3] flakes were prepared using a modified Hummers method and dispersed in water with a concentration of 0.5 mg/mL. The samples were prepared by drop casting, the GO and DNA with buffered solution [1] on 300 nm SiO_2 /Si(100) at room temperature. AFM image of the GO flakes,) shows the typical AFM image of the DNA-GO complex, where the bright areas on the GO surface might be due to the adsorption of DNA. In this complex the thickness is about 3 nm.This observation indicates that GO can strongly adsorb ssDNA and can efficiently quench its fluorescence. The fluorescently labeled ssDNA-GO complex displayed significant fluorescence enhancement upon addition of complementary target DNA oligonucleotide (Figure 1b). This recovery of fluorescence increases with increasing concentration of the target DNA added to the mixture.

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3. Perrozzi F.; et al.; J. Phys.: Condens. Matter 27, 013002 (2015) doi:10.1088/0953-8984/27/1/013002 Graphene oxide: from fundamentals to applications.

Strain-free structural transition during Li-ion roching chair battery operation based on LTO anodes

Sikandan A.[1], *Asif M.*[1], *Gunnella R.*[1], *Nobili F.*[2], *Calcaterra S.*[2], *Pasqualini M.*[2], *Rezvani S.J.*[1], *Ciambezi M.*[1], *Di Cicco A.*[1]

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LTO ($Li_4Ti_5O_{12}$) spinel to cubic transformation [1] induced by Li insertion in octahedral sites and concomitant migration of pristine lithium from tetrahedral sites, is in principle strain-free; correspondly can guarantee a longer life-time and cyclability, in spite of a lower energy density, for higher frequency applications. The transformation to a cubic structure though apparently does not affect the volume, creates at the level of the surface a strong rearrengement of the electrode changing morphology and chemical composition [2], that can exceed the theoretical capacitance [3]. The structure of the device is controlled, during batteries charge and discharge cycles, at the atomic level as a function of time by using XAS [4], a chemical sensitive and short range probe, and by selectively tuning the detection depth by collecting electrons, total and partial yield, and photon fluorescence yield. X-ray absorption experiments have been conceived and realized to study the modification of the signals related to the various atomic species in LTO electrodes selected at different states of charge during the first Li insertion process and thickness. In particular the comparison with multiple scattering models including inverted spinel transformation and Li_2TiO_3 reversible growth on the electrodes was able to pin critical transition and surface layer modification that can be additional sources of capacity of the device. Furthermore the instability of the highly reactive oxide since the initial pristine material conditions was critically discussed.

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Investigating Italian science teachers' transformations while implementing inquiry teaching learning-sequences

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Scientific Inquiry (SI) is nowadays considered an essential component of scientific literacy[1]. In such approaches, methods of inquiry used by students resemble the way in which professional scientists and researchers carry out their work[2]. However, research studies have shown that when implementing innovative teaching-learning approaches, even trained teachers can "transform" the original designers' objectives[3]. While some transforming trends may lead to fruitful modifications, others may impact in a negative way, leading, in some cases, to substantial modification in the enactment of curriculum materials. This research study aims to investigate the mostly transformed/accepted aspects of scientific inquiry, while it is implemented in classroom practice. Twenty secondary school science teachers were involved in a thirty-hours professional development (PD) course on IBSE, aimed to familiarize them with inquiry principles using seven teaching learning-sequences[4] as training contexts. Then, teachers implemented one TLS in their classrooms. A knowledge transfer framework, Adaption and Re-Invention Model[5], was used to investigate teachers' transfer of TLS in classroom practice. In particular, core and non core elements of the TLSs were identified: core elements are essential features of inquiry teaching that should not be changed while implementing a TLS. Non core elements concern classroom management and activities timing and can be changed to fit the TLS into the specific educational context. Collected data have been audio/video recordings. Results show that most accepted aspects of inquiry teaching are related to data collection, support to students, activities timing and homework tasks. Moreover, most teachers acted as resource persons and valued classroom discussions. Findings also provide evidence of how teachers enact inquiry teaching in their practice and may usefully inform PD courses.

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