

PhD Day⁶

The day dedicated to the PhD students



Abstract booklet

27th May 2015



UNIVERSITÀ
DEGLI STUDI
FIRENZE

PhD - Day⁶

Academic cooperation is of great importance in creating a research network between colleagues from different fields of study. An interuniversity research network is indeed fundamental for both the quantity and quality of the research production. During the PhD-Day⁶, participants will present their research work and discuss their findings as well. Moreover, researchers and PhD students will have the opportunity to meet each other, communicate about interesting topics, share ideas and information, hopefully leading to new collaborations. On the other hand, undergraduate students can learn more about topics usually not covered during the course of studies. Finally, PhD-Day⁶ is a good opportunity for students, who need to choose their thesis, to gain understanding of different research groups and their research project!

Sessions

The following sessions collect the contributions of PhD students belonging to 16 different PhD courses and much more curricula and 17 Departments. Due to the high number of participants, the diversity and amount of different topics, the talks are organized in 8 thematic sessions that will be held in 3 parallel sessions.

Drugs and Health

From the development of new diagnostic approaches to the synthesis of specific drugs and new delivery systems for a targeted therapy of diseases. A mystic trip in the Health care Universe.

International Year of Light

Special session dedicated to the Unesco “International Year of Light”. Many topics, ranging from atomic physics to photonics and astrophysics, but with one point in common: light.

Engineering, Informatics and Statistics

An exciting tour from space to the details contained in the human genome.

Cellular Biology

From proteins to hormones and ions for diagnosis and therapy. The cellular biology revealed for a better understanding of quite rare and immunological diseases.

Neuroscience

Tackling one of the most difficult questions on the human being: what's going on in the nervous system? From the understanding of the basic functioning of the human mind to the active research of the causes and treatments for some of humanity's most disabling disorders.

Magnetism

From theoretical studies to single molecule magnets for experimental purposes. The magnetism as a powerful force in the material science field.

Environment and Cultural Heritage

A mixture of Earth and human products: from the study of the environment, climate and animals to the conservation of cultural heritage and the production of eco-sustainable resources.

Poster Session

The Poster Session is a privileged moment. It is a space that allows direct comparison, exchange of ideas and information with the authors. Posters will be displayed throughout the day and will have two dedicated moments: a short one during the coffee break in the morning and one in the afternoon session. During the completion of the work will be rewarded posters chosen by you. Do not forget to express your preferences at the table in front of the Aula Magna. – *thanks to google translate ;-)*

Programme at a glance

8:30

**Welcome
and
Registration**

Dean's Opening Speech
Prof. Alberto Tesi

Aula Magna

10:00

Plenary Session

Aula Magna

10:45

Coffee Break

11:30

Drugs & Health

Aula 35

Intern. Year of Light

Aula Magna

Eng., Inf. & Stat.

Aula 36

13:00

Time for Lunch

14:15

**Cellular Biol.
Neuroscience**

Aula 35

Intern. Year of Light

Magnetism

Aula Magna

Envir. & Cultural Heritage

Aula 36

17:00

**Poster Session
and
Coffee Break**

18:00

**Conclusion
and
Poster Award**

Aula Magna

Talks

Plenary Session

Aula Magna

10:00 - T-1: *Optically tunable polymeric photonic structures*

Sara Nocentini

10:15 - T-2: *Is motor imagery already present before age of 5? A pilot action research study*

Francesco Di Gruttola

10:30 - T-3: *E-ELT HIRES science case for astrobio logical relevant targets: new comets*

Sara Faggi

Drugs & Health

Aula 35

11:30 - T-4: *War against cancer*

Tiziano Marzo

11:45 - T-5: *Fabrication of gold nanorods for
incorporation into nanocapsule systems for drug
delivery*

Federica Scaletti

12:00 - T-6: *The PI3K inhibitors BEZ235 and
RAD001 are effective against JAK2V617F mutated
cells and synergize with ruxolitinib in preclinical models*

Serena Martinelli

12:15 - T-7: *Characterization of CALR mutations
in patients with chronic myeloproliferative neoplasms*

Laura Calabresi

12:30 - T-8: *Functional defects of T-tubular system
in a transgenic model of hypertrophic cardiomyopathy*

Marina Scardigli

12:45 - T-9: *The gut microbiota and mycobiota in
health and disease*

Monica Di Paola

International Year of Light (1)

Aula Magna

11:30 - T-10: *Near-field mapping of TE and TM modes in silicon microrings*

Federico La China

11:45 - T-11: *The Beetle's white album*

Lorenzo Cortese

12:00 - T-12: *How to cook your own Pulsar Wind Nebula*

Barbara Olmi

12:15 - T-13: *Tracking light transport at a trillion frames per second: non-linear optical gating applications beyond Diffusion theory*

Lorenzo Pattelli

12:30 - T-14: *Twisted magnetosphere in general relativistic neutron stars*

Antonio Pili

12:45 - T-15: *Integration of carbon nanotubes on silicon photonic structures for efficient emission at telecom wavelengths*

Francesco Sarti

Engineering, Informatics & Statistics

Aula 36

11:30 - T-16: *The Decommissioning Device: a
technology for a sustainable access to space*

Alessio Fanfani

11:45 - T-17: *Ultrasound system for in-line
industrial applications*

Valentino Meacci

12:00 - T-18: *Understanding the small group
processes on computer-mediated collaborative learning*

Elisa Guidi

12:15 - T-19: *MeDuSa: a multi draft based
scaffolder*

Emanuele Bosi

12:30 - T-20: *Novel ultrasound method for accurate
blood velocity measurement*

Riccardo Matera

12:45 - T-21: *A contribution to the development of high school geometry teaching based on computer formalization with a constructive approach*

Mohamed Rabii Kadib Alban

Cellular Biology

Aula 35

14:30 - T-22: *Just a flexible linker? The structural and dynamic properties of CBP-ID4 as revealed by NMR spectroscopy*

Alessandro Piai

14:45 - T-23: *Study of the conformational changes occurring in human transthyretin that are necessary for amyloid fibril formation in disease and for its role as a detoxifier*

Seyyed Abolghasem Ghadami

15:00 - T-24: *Understanding the molecular mechanism of the maturation of cytosolic Iron-Sulfur cluster proteins*

Riccardo Muzzioli

15:15 - T-25: *[2Fe-2S] BolA3-GLRX5: a novel player in ISC assembly machinery*

Veronica Nasta

15:30 - T-26: *Structural and morphological investigation of TDP-43 aggregates*

Claudia Capitini

Neuroscience

Aula 35

15:45 - T-27: *Dissecting brain architecture with a new clearing method*

Antonino Paolo Di Giovanna

16:00 - T-28: *Evaluation of secretases activity in Alzheimer's disease with fluorescent probes*

Niccolò Parenti

16:15 - T-29: *Oleuropein aglycone in the TgCRND8 mouse model of A β deposition*

Pamela Nardiello

16:30 - T-30: *miRNA in Amyotrophic Lateral Sclerosis: pathogenic role and potential biomarkers*

Michele Benigni

16:45 - T-31: *Molecular and genetic analysis of OPA1, CAPN3 and DYSF gene*

Sara Aguti

International Year of Light (2)

Aula Magna

14:15 - T-32: *Single-molecule study for a graphene-based nano-position sensor*

Giacomo Mazzamuto

14:30 - T-33: *Raman measurements of hydrogen clathrate hydrate synthesized from liquid*

Leonardo del Rosso

14:45 - T-34: *Universal state orthogonalizer and qubit generator*

Luca Costanzo

15:00 - T-35: *Can a superfluid in one dimension flow without dissipation?*

Simona Scaffidi Abbate

15:15 - T-36: *3D Anderson localization with ultracold atoms*

Giulia Semeghini

15:30 - T-37: *QCL-based metrological-grade THz spectroscopy tools*

Annamaria Campa

15:45 - T-38: *Coevolution Black Holes and host galaxies*

Stefano Carniani

Magnetism

Aula Magna

16:00 - T-39: *Dy(LH)₃dmf complex: a multitechnique approach for a meaningful magnetic characterisation*

Eva Lucaccini

16:15 - T-40: *Assembling Fe₄ Single Molecule Magnets: paving the way to molecular spintronics*

Irene Cimatti

16:30 - T-41: *Exchange bias in Co_xFe_{1-x}O(AFM)|Co_xFe_{3-x}O₄(FiM) Core/Shell nanoparticles*

Elisabetta Lottini

16:45 - T-42: *Mapping the spin structure of a chiral magnet*

Mauro Perfetti

Environment & Cultural Heritage

Aula 36

14:30 - T-43: *Mo and stable U isotopes as tracers for subduction components in the Quaternary West-Mediterranean potassic and ultrapotassic magmatism*

Martina Casalini

14:45 - T-44: *A simplified procedure to assess 1D seismic response in Tuscany Region*

Giacomo Peruzzi

15:00 - T-45: *Preliminary studies of GV7, a new drilling site in East Antarctica*

Laura Caiazzo

15:15 - T-46: *Energy, hydrogen and chemicals by renewable alcohols electrooxidation*

Marco Bellini

15:30 - T-47: *Investigation of the structural properties of MgO-based eco-sustainable cements*

Monica Tonelli

15:45 - T-48: *Good vibrations: the role of substrate-borne vibrations in mating behaviour of the leafhopper *Empoasca vitis**

Rachele Nieri

16:00 - T-49: *Copulatory success in lekking fallow (*Dama dama*) bucks: hypotheses testing using generalized structural equation models*

Sonia Lombardi

16:15 - T-50: *Qualification and traceability of Tuscany milk through NMR-based metabolomics*

Claudio Santucci

16:30 - T-51: *Multivariate analysis of combined first-derivative micro-Raman and reflectance FT-NIR spectra for the analysis of binder materials both neat and in simulated mixtures*

Serena Carlesi

16:45 - T-52: *Conservation and restoration of archaic stones of ancient cities of Euromos and Iasos Turkey*

Halit Canol

Talk abstracts

Talk

Ciclo XXIX

Optically tunable polymeric photonic structures

Sara NocentiniINTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS -
Laboratorio Europeo di Spettroscopia non Lineari (LENS)

MATERIAL SCIENCE, OPTICS AND PHOTONICS, POLYMER SCIENCE

Integrated optical polymeric components have already been chosen in optical communication for their high bandwidth, low-cost and good integration with the existing silicon photonic technologies. A higher degree of integration, than the planar fabrication approach, can be achieved through the dip-in direct-laser-writing (DLW) lithographic technique that allows fabricating three-dimensional polymeric devices. Exploiting this technique, we present a 3D integrated polymeric circuit on a glass substrate constituted by waveguides, whispering gallery mode resonators and interferometers.

Moreover reversible and stable tuning of the optical properties is an important achievement that provides a higher level of functionality. Reliable tunability has been achieved through the integration of liquid crystalline elastomeric (LCE) structures realized in a second step process with the DLW technique. The optical response of the elastomer allows reshaping the photonic components leading to the remote control of the photonic properties. We demonstrate the tuning of the lasing modes, over a large spectral range, of a whispering gallery mode resonator micro-laser integrating a LCE cylinder on the top of the cavity. This way of optical tuning creates interesting different possibilities for all-optical control of the photonic properties in integrated circuits.

Talk

Ciclo XXX

Is motor imagery already present before age of 5? A
pilot action research study

Francesco Di Gruttola

DOTTORATO TOSCANO DI NEUROSCIENZE - Dipartimento di Ricerca traslazionale e
delle nuove tecnologie in Medicina e Chirurgia (Università di Pisa)

NEUROSCIENCE, SPORT PSYCHOLOGY

Motor Imagery (MI), that is the ability to mentally rehearse motor acts without overt body movements, is an important acquisition for children to learn, program and control movements. There are evidences that this capacity is present from the age of 5, but there are only few studies with children under 7 years old. This because of some theoretical and methodological problems. In this regard, we longitudinally studied 16 children from 2 to 3 and 6 months years old during a two months psychomotor intervention dividing them into a MI and a visual imagery (VI) group respectively, automatically evoking these abilities with short stories. To assess motor, cognitive, social and linguistic development of children we used the “Ages and Stages Questionnaire - Third Edition” (ASQ-3) completed by parents twice in total, before the start of the intervention and immediately after the end. The research will be completed in late April 2015, but we expect a significant improvement in the development of motor and cognitive skills of children who take part in the MI than in the VI condition as evidence of the MI presence also in very young children.

Talk

Ciclo XXIX

E-ELT HIRES science case for astrobio logical relevant targets: new comets

Sara Faggi

DOTTORATO IN FISICA E ASTRONOMIA - Astronomia - Dipartimento di Fisica e
Astronomia

SPECTROSCOPY, ASTROPHYSICS

New comets are comets coming from the Oort Cloud at their first passage close to the Sun. They are particularly important because they are supposed to have a large quantity of fresh (not processed) organic matter close to the surface. Comets are among the most pristine bodies of the solar system and their study can give precious informations on the formation of the Solar System itself. Moreover, they probably played an important role in depositing the organic matter that, 4.6-3.6 Gyr ago, contributed to the appearance of life on the primordial Earth. High-resolution spectroscopy in the near-infrared spectral range is a powerful tool for chemical abundances studies. In the spectra of cometary comae there are a lot of molecular bands and their ro-vibrational structures are useful to investigate the physical conditions of their coma. To understand how to study new comets in the (0.37-2.5) μm spectral range with HIRES, we are planning an observation campaign with GIANO, high resolution spectrograph in the (0.95-2.45) μm spectral range, at TNG. The opportunity to observe with GIANO would allow us to plan the best use of new IR-high resolution spectrographs, like HIRES, on 30 m class telescope as EELT.

Talk

Ciclo XXVIII

War against cancer

Tiziano Marzo

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

INORGANIC CHEMISTRY, DRUGS-HEALTH, MEDICINAL CHEMISTRY

Great War has been one of the most dramatic event in our history. The high number of victims, directly or indirectly determined by the conflict are imputable, for a large part, to the new military strategies and to the new weapons. New technologies provided an incredible and unexpected destructive potential. Within this frame scientists played a key role and the widespread use of chemical warfare has been a peculiar feature of WW1. Chemists rapidly developed a series of gases such as phosgene and mustard gas, capable to react with biological molecules (including DNA), and to cause severe (and often irreversible) damage to the eyes, respiratory system and internal organs, also with fatal consequences. Remarkably, in those years, scientists realized that Bis(2-chloroethyl) sulfide (i.e. mustard gas or iprit) was a strong suppressor of hematopoiesis and able to reduce white blood cells counts. Since white blood cells reproduce with high rate, similarly to cancer cells, they started to hypothesize a possible use of this class of molecules as chemotherapeutic agents, to fight cancer; was the born of chemotherapy. History tells us that these observations have been of great impact and importance, leading to development of modern and more effective anticancer agents. Despite progresses in this field, still, heavy side effects and resistance to the drugs, represent serious drawbacks to be overcome.

Talk

Ciclo XXVII

Fabrication of gold nanorods for incorporation into nanocapsule systems for drug delivery

Federica Scaletti

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

MATERIAL SCIENCE, GOLD NANORODS, NANOCAPSULE, DRUG DELIVERY

Gold nanorods (GNRs) have attracted a widespread attention due to their tremendous potential for biomedical applications, from the detection of protein/DNA interactions to drug delivery, cancer therapeutics and diagnostics. Specifically GNRs exhibit unique optical properties, which include a surface plasmon absorption band in the visible region and a second tunable absorption in the NIR, making them good agents for both therapy and diagnosis. In particular small sized gold nanorods, showing a longitudinal plasmon absorption in the near-infrared window (700-900 nm), are of great interest for potential *in vivo* applications (e.g., photothermal therapy) and for their high-payload-to-carrier ratio (e.g., drug delivery). In the present work GNRs were fabricated and properly functionalized to allow them to incorporate into nanocapsule systems for drug delivery. GNRs were assembled at the interface of an oil-in-water emulsion to combine the delivery of hydrophobic drugs and the optical properties of GNRs. The synthesis of GNRs was modified to obtain small gold nanorods and the preparation of the nanocapsules was optimized for the realization of nanocapsules with a size for an optimal activity as drug delivery system. The plasmonic properties of GNRs were determined and the stability of the nanocapsules in physiological condition was evaluated. Therefore the nanocapsule's application as drug delivery system was explored using cell culture models.

Talk

Ciclo XXVII

The PI3K inhibitors BEZ235 and RAD001 are effective against JAK2V617F mutated cells and synergize with ruxolitinib in preclinical models

Serena Martinelli

DOTTORATO IN SCIENZE BIOMEDICHE - Oncologia Sperimentale e Clinica -
Dipartimento di Medicina Sperimentale e Clinica

DRUGS-HEALTH, PHARMACOLOGY

Janus kinase 2 mutation (JAK2V617F) represents the molecular alteration of the majority of chronic myeloproliferative neoplasms (MPN). Enhanced activation of other downstream pathways including the PI3K/mTOR has been documented as well. Targeting mTOR by RAD001 resulted in inhibition of JAK2V617F mutated cells. We evaluated the effects of BEZ235, a PI3K inhibitor, alone and in combination with mTORC1 (RAD001) and JAK2 (ruxolitinib) inhibitor in MPN models. We found that BEZ235 preferential inhibited murine and human JAK2V617F mutated cell lines compared to WT counterpart. BEZ235 significantly induced cell cycle arrest in G2/M phase and induced apoptosis. Western blot showed reduction of phospho-mTOR and phospho-4EBP1 as well as down-regulation of phospho-STAT5. BEZ235 impaired colony formation from patients CD34+ cells at doses 2 to 8-fold lower than controls. Triple combination including BEZ235/ruxo/RAD001 resulted highly synergistic *in vitro* and in KI mice induced reduction of leukocytosis, reticulocyte count and improvement of splenomegaly: the level of phospho-STAT5 and phospho-4EBP1 in the spleen was significantly reduced in mice receiving triple-treatment compared to single drug treatment. Inhibition of PI3K and JAK2 pathways resulted in anti-tumor activity in preclinical models of JAK2V617F mutated MPN and provide a rationale for future combination clinical trials.

Talk

Ciclo XXX

Characterization of CALR mutations in patients with chronic myeloproliferative neoplasms

Laura Calabresi

DOTTORATO IN SCIENZE BIOMEDICHE - Oncologia Sperimentale e Clinica -
Dipartimento di Medicina Sperimentale e Clinica
DRUGS-HEALTH, PHARMACOLOGY, CELLULAR BIOLOGY

Chronic myeloproliferative neoplasms (MPN) include Polycythemia Vera (PV), Essential Thrombocythemia (ET) and Primary Myelofibrosis (PMF). About 60 % of the patients harbor JAK2V617F and MPL mutations. We contributed to the discovery of calreticulin mutations (CALRmut) in 60-80 % of JAK2/MPL-negative patients with ET and PMF. This represents a significant improvement for diagnosis. CALR mutations are heterogeneous spanning over the exon 9, but all result in a novel common protein C terminus. We developed a polyclonal antibody against a 17-amino-acid peptide derived from mutated calreticulin that was used for immunostaining of bone marrow biopsies. We show that this antibody specifically recognized patients harboring different types of CALR mutation with no staining in healthy controls and JAK2- or MPL-mutated ET and PMF. The labeling was mostly localized in megakaryocytes, whereas myeloid and erythroid cells showed faint staining, suggesting a preferential expression of calreticulin in megakaryocytes. Megakaryocytic-restricted expression of calreticulin was also demonstrated using an antibody against wild-type calreticulin and by measuring the levels of calreticulin RNA by gene expression analysis. Immunostaining using an antibody specific for mutated calreticulin may become a rapid, simple and cost-effective method for identifying CALR-mutated patients complementing molecular analysis; furthermore, the labeling pattern supports the preferential expansion of megakaryocytic cell lineage as a result of CALR mutation in an immature hematopoietic stem cell.

Talk

Ciclo XXX

Functional defects of T-tubular system in a transgenic model of hypertrophic cardiomyopathy

Marina Scardigli

DOTTORATO DI RICERCA IN MEDICINA MOLECOLARE (UNIVERSITÀ DI SIENA) -
Laboratorio Europeo di Spettroscopie non Lineari (LENS)

MICROSCOPY, BIOPHYSICS, CELLULAR BIOLOGY

T-tubules constitute a complex system of membrane invaginations that allow a uniform propagation of action potential in cardiac cells. Alterations of T-tubules is reported in several cardiac diseases but little is known about hypertrophic cardiomyopathy (HCM), the most prevalent monogenic disorder in humans. The aim of this study is to correlate the role of the T-tubular system to the electrical dysfunction in a cTnT mutation associated with HCM. We employ a mouse model of HCM carrying the $\Delta 160E$ cTnT mutation, compared with wild type siblings, to assess the electrical function of the tubular compartment. A two-photon random access microscope is employed to dissect the spatio-temporal relationship between T-tubular electrical activity and Ca^{2+} release in isolated cardiomyocytes. In cTnT $\Delta 160E$ cardiomyocytes, we find a significant number of T-tubules failing to propagate action potentials, with consequent delay of local Ca^{2+} release. At variance with wild type, we also observe significantly increased variability of Ca^{2+} transients as well as higher Ca^{2+} -spark frequency. Although T-tubule structural remodeling in cTnT $\Delta 160E$ myocytes is modest, the measured functional defects determine non-homogeneous Ca^{2+} release and delayed activation of the contractile machinery, explaining the pathological contractile dysfunction.

Talk

Ciclo XXIX

The gut microbiota and mycobiota in health and disease

Monica Di Paola

DOTTORATO INTERNAZIONALE IN AREA DEL FARMACO E TRATTAMENTI INNOVATIVI
- Farmacologia, Tossicologia e Trattamenti Innovativi - Dipartimento di Neuroscienze,
Psicologia, Area del Farmaco e Salute del Bambino (NEUROFARBA)

PHARMACOLOGY, MICROBIOLOGY, METAGENOMICS, NUTRITION

The gastrointestinal tract harbours a complex community of microbes. The commensal bacteria, the microbiota, and fungi, the mycobiota, play a fundamental role in controlling many aspects of host physiology, such as production of energy and nutrients and detoxification processes. The relationship between the gastrointestinal tract and resident microbiota and mycobiota is complex and multifaceted. Bacteria and Fungi co-evolved with their host and together they are active participants influencing health and disease. The mucosal immune system has developed specialised regulatory and anti-inflammatory mechanisms for eliminating or tolerating commensal microorganisms. Dysregulations of the gut immune response to commensal Bacteria and Fungi play a crucial role in chronic inflammatory and autoimmune diseases. In this study, we characterized the gut communities in healthy subjects and in gastrointestinal diseases, such as Inflammatory Bowel Diseases. We will show that, on the one hand, alteration of microbiota (dysbiosis) plays an important role in chronic inflammatory disease and, on the other hand the mycobiota contributes to worsen the inflammatory response, leading to increased disease severity. Understanding the contribution of the microbiota and mycobiota and their shaping and adaptation in the gut might lead to novel approaches to prevent and manage chronic gastrointestinal disease.

Talk

Ciclo XXIX

Near-field mapping of TE and TM modes in silicon microrings

Federico La China

INTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS -
Laboratorio Europeo di Spettroscopie non Lineari (LENS)

SPECTROSCOPY, OPTICS AND PHOTONICS

We present a deep sub-wavelength imaging of the modes localized in silicon microring resonators, obtained by combining near-field scanning optical microscopy with resonant scattering spectroscopy. We use resonant forward scattering geometry with polarization control to get a hyperspectral mapping of both TE and TM modes, without the need of evanescent coupling with a waveguide. The simultaneous analysis of spatial maps and spectral lineshapes gives a clear understanding of the mode nature. Polarization control imaging of the different spatial distribution of the TE and TM modes allows us to clearly identify the two mode families. We demonstrate that both TE and TM modes have in-plane electric field polarization few nm outside the ring, suggesting that the microring may be of the utmost relevance for coupling them to external emitters, such as quantum dots, molecules or carbon nanotubes.

Talk

Ciclo XXVIII

The Beetle's white album

Lorenzo Cortese

INTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS -
Laboratorio Europeo di Spettroscopia non Lineari (LENS)

SPECTROSCOPY, OPTICS AND PHOTONICS, MATTER PHYSICS, DISORDERED
PHOTONICS, DIFFUSION OF LIGHT, BIO-INSPIRED PHOTONICS

The colours shown by several insects often arise from light scattering by very complex photonic structures rather than selective absorption by pigments. Such structures are the result of optical strategies developed during millions of years of evolution. The bright and iridescent colours shown by certain butterflies and beetles, for example, arise from coherent effects which requires ultrathin periodic layers of material. In contrast, a bright white colouration is more complicated to achieve, since all colours has to be scattered with the same high efficiency. In this case the wave nature of light is not involved in the appearance of the object, and a bright white is achieved only in presence of multiple scattering, for which thicker, high-refractive-index contrast systems are usually required. Nevertheless, the extremely brilliant whiteness shown by the *Cyphochilus* beetle is generated light scattering inside the ultra-thin scales that cover its body. The intra scale structure is characterized by a dense, nanostructured network of low-refractive-index chitin filaments, which seems to be optimised (during millions of years of evolution) to increase the total reflectance, and thus the bright appearance of the beetle, employing as less material as possible. In this work, through an experimental study of light transport inside the beetle scales, we unveil the crucial aspects of such optical optimisation carried on by evolution.

Talk

Ciclo XXVIII

How to cook your own Pulsar Wind Nebula

Barbara OlmiDOTTORATO IN FISICA E ASTRONOMIA - Astronomia - Dipartimento di Fisica e
Astronomia

COMPUTATIONAL MODELING, FLUID DYNAMICS, ASTROPHYSICS

Pulsar Wind Nebulae (PWNe) are a particular class of supernova remnants, produced in the violent death of a massive star as a supernova explosion. They show a fill centered emission morphology, that arise from the interaction of the relativistic wind emanating from the rapidly rotating neutron star with its surroundings. The study of these objects is currently of great interest: since PWNe are candidates to be among the primary antimatter factories in the Galaxy, they can be the reason behind the positron excess recently measured by Pamela and AMS02; they are also one of the most powerful accelerators known, being able to accelerate particles up to PeV energies. Unfortunately the region that probably holds the fundamental informations on the physics behind the acceleration and particle creation mechanisms, the pulsar wind, is not able to emit any electromagnetic radiation and it is thus not directly observable.

The only way we do have to inspect the wind nature is to build a theoretical model and let it evolve using numerical simulations. I will illustrate a possible PWN recipe, from the fundamental ingredients to the final object.

Talk

Ciclo XXIX

Tracking light transport at a trillion frames per second:
non-linear optical gating applications beyond Diffusion
theory

Lorenzo Pattelli

INTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS -
Laboratorio Europeo di Spettroscopia non Lineari (LENS)

OPTICS AND PHOTONICS, ULTRAFAST IMAGING, NON-LINEAR OPTICAL GATING,
LIGHT TRANSPORT IN TURBID MEDIA

Accessing the spatial evolution of a physical phenomenon with high temporal resolution is often the key to reveal its basic principles. Dealing with light transport in disordered media, the ability to track light's spatio-temporal spreading can bring a wealth of information regarding their chemical, physical and structural properties. In such media, light can be regarded as a particle flux, since multiply scattered light quickly loses its phase coherence. Even so, many aspects of light transport still elude our comprehension, and the applicability of Diffusion Theory is continuously and actively debated. Experimentally, several detection techniques such as streak cameras are inherently limited by their electronic circuitry setting a lower bound to the time (and therefore spatial) scale on which light transport can be investigated. On the contrary, many interesting samples such as biological tissues come in a limited range of sizes, not to mention the fundamental interest raised by sub-ps light transport itself. In this talk, I will give a short introduction on optical gating techniques and their ultra-fast imaging applications. On a sub-ps time scale, a whole new range of samples (in terms of both size and opacity) can be investigated: in doing so, we were able to address a new transport regime where Diffusion theory is no longer applicable despite the onset of multiple scattering.

Talk

Ciclo XXIX

Twisted magnetosphere in general relativistic neutron stars

Antonio Pili

DOTTORATO IN FISICA E ASTRONOMIA - Astronomia - Dipartimento di Fisica e
Astronomia

COMPUTATIONAL MODELING, HIGH ENERGY ASTROPHYSIC

The phenomenology of the emission of magnetars supports the idea that their magnetosphere are tightly twisted in the vicinity of the star. I will discuss the properties of equilibrium models of magnetized neutron stars endowed with a twisted magnetosphere obtained solving the general relativistic Grad–Shafranov equation, both in the interior and in the exterior of the star.

Talk

Ciclo XXIX

Integration of carbon nanotubes on silicon photonic structures for efficient emission at telecom wavelengths

Francesco Sarti

INTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS -
Laboratorio Europeo di Spettroscopie non Lineari (LENS)

OPTICS AND PHOTONICS, MATTER PHYSICS

Information and Communication Technologies require efficient optoelectronic devices integrated on Si substrates to emit light. Since Si is an indirect-bandgap material, the insertion of efficient emitters is required. We investigated the use of carbon nanotubes (CNT) at the telecom wavelength range (1300 nm and 1500 nm). After theoretical calculations we chose PFO polymer for the HiPCO nanotubes and PFH-A polymer for laser ablation nanotubes. Different purification protocols in toluene have been investigated to optimize the radiative efficiency. Detailed analysis by means of absorption, photoluminescence (PL), photoluminescence excitation and Raman show the very small contamination (if any) of metallic CNTs, the improved concentration of semiconducting CNTs, the small concentration of bundle, the narrow spectral broadening and the small concentration of the unused polymer. We deposited these CNTs solutions on different substrates: quartz, Si and SiN₄. High-resolution PL measurements show bright emission in the near infrared and high-resolution PL mapping allows to determine the CNT areal density, the spatial distribution features and single CNT PL emission. CNT integration on Si slot-microring resonators has been also realized. We observed sharp peaks due to the CNTs PL coupling to microrings. Our results pave the way to establish the potential of CNT technology for nanophotonic applications.

Talk

Ciclo XXIX

The Decommissioning Device: a technology for a sustainable access to space

Alessio Fanfani

DOTTORATO IN INGEGNERIA DELL'INFORMAZIONE - Telecomunicazioni -
Dipartimento di Ingegneria dell'Informazione (DINFO)

ENVIRONMENTAL / POLLUTION, INDUSTRIAL ENGINEERING, SATELLITE
COMMUNICATION

The most interesting orbits for space activities, as GEO and LEO ones, are getting crowded by an huge number of space debris. They are man-made objects like as dead satellites, upper stages, pieces from fragmentation or collision. The number of that space debris is higher than some hundred million and it represents one of the most severe threats to a sustainable access to space for humanity in the next future. With the objective to contribute solving this problem, D-Orbit is developing a Decommissioning Device to be used for debris mitigation purposes on newly-launched space systems by allowing a safe, quick post-mission disposal. A key element of the Decommissioning Device is the telecommunication system that provides a reliable link also when the satellite has limited functionalities, with a random and uncontrollable attitude or is defunct. Different solutions could be suitable depending on the satellite mission. In Decommissioning Device for LEO nanosatellite, an actual example is the D-SAT satellite scheduled for launch in the 2016, an omnidirectional antenna allows to use traditional communication techniques. Otherwise, in a scenario with bigger satellites and higher orbits, new transmission techniques has to be investigated.

Talk

Ciclo XXIX

Ultrasound system for in-line industrial applications

Valentino Meacci

DOTTORATO IN INGEGNERIA DELL'INFORMAZIONE - Elettronica ed
Elettromagnetismo - Dipartimento di Ingegneria dell'Informazione (DINFO)

INDUSTRIAL ENGINEERING, ELECTRONIC EMBEDDED SYSTEMS

The in-line measurement of the properties of fluids is crucial in chemical, cosmetic, pharmaceutical, and food industries in order to optimize the production process and improve the product quality. An Ultrasound system uses the Doppler effect in order to investigate the velocity of fluid in a process pipe and to obtain the properties of fluid by means a mathematical model. In this work, we present a compact and fully programmable low-cost Ultrasound system, specifically design for industrial use, where all of the electronics necessary for controlling the probe and elaborating the signals is embedded in a compact board. The system produces the transmission signal, and amplifies, converts and elaborates the received echoes for obtaining the velocity profile (VP). The VP data are stored in a memory and downloaded by an Ethernet interface. This system is perfectly fits industrial applications thanks to the full programmability of the parameters and the capability of elaborating large amounts of data.

Talk

Ciclo XXIX

Understanding the small group processes on computer-mediated collaborative learning

Elisa Guidi

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Complessi - Dipartimento di Ingegneria dell'Informazione (DINFO)

COMPUTATIONAL MODELING

In today's world, the use of information and communication technologies (ICTs) to assist learning processes is on the increase. One of the main purposes of ICT use in learning processes is to facilitate collaboration and, therefore, improve learning by means of sharing and distributing knowledge. This paper describes a study aimed to investigate the effects that a small group has on the individual and collaborative learning. In our study, a chat was used to simulate a virtual environment (VE), which allowed us to study the dynamics of human social behavior. Our results seems to support the hypothesis that even in virtual environments are functioning social scripts in the interaction between individuals, or it is possible to develop social strategies for problem solving. This study, combined with the chat content analysis, may suggest useful advices about collective reasoning and e-learning dynamics, which are nowadays very relevant topics in the study of web communities and educational communities.

Talk

Ciclo XXVIII

MeDuSa: a multi draft based scaffold

Emanuele Bosi

DOTTORATO IN SCIENZE E TECNOLOGIE VEGETALI, MICROBIOLOGICHE E GENETICHE - Scienze Genetiche, Microbiologiche e Bioinformatica - Dipartimento di Biologia (BIO)

ECOLOGY / ETHOLOGY / EVOLUTION, BIOINFORMATICS, GENOMICS

Completing the genome sequence of an organism is an important task in comparative, functional and structural genomics. Nevertheless, this is still a challenging issue, from both computational and experimental viewpoints. Genome scaffolding (i.e. the process of ordering and orientating contigs) originated from *de novo* assembly is usually the first step in common genomes finishing pipelines. We developed and implemented a method for genome scaffolding called MeDuSa (Multi Draft based Scaffold), which exploits the information present in the sequence of phylogenetically related genomes to scaffold to obtain scaffolds. The tool has been benchmarked against other tools present in the field and it has been found how MeDuSa outperforms the other methods in accuracy, running time and usability.

Talk

Ciclo XXVIII

Novel ultrasound method for accurate blood velocity measurement

Riccardo Matera

DOTTORATO IN INGEGNERIA DELL'INFORMAZIONE - Elettronica ed
Elettromagnetismo - Dipartimento di Ingegneria dell'Informazione (DINFO)

DRUGS-HEALTH, ULTRASOUND METHODS

Ultrasound echographs are routinely used in clinical practice for their safety, reduced cost, and image quality. In particular, Doppler ultrasound delivers important information about how the blood moves in arteries and veins. During the exam the echograph transmits a sequence of energy bursts at a known frequency along a single direction that intersects in the vessel to be investigated. According to the Doppler effect, the blood particles reflect the ultrasound wave with a frequency shift that is proportional to the particle velocity and the angle between the incident wave and the velocity direction. The echograph, reading the frequency shift, calculates the blood velocity and shows it in a display. The peak velocity of the blood is an important medical parameter assessed during this exam. For example, it is used to evaluate the grade of a stenosis, i.e. the pathological narrowing that reduces the lumen of an artery. Unfortunately, the method currently used for the blood peak detection, as reported by major medical literature, is widely inaccurate and operator dependent. In this work a novel Doppler ultrasound method, based on the transmission of pulses of particular shape and from different directions, is shown to produce more accurate measurements.

Talk

Ciclo XXVII

A contribution to the development of high school
geometry teaching based on computer formalization
with a constructive approach

Mohamed Rabii Kadib Alban

DOTTORATO IN MATEMATICA, INFORMATICA, STATISTICA - Matematica -
Dipartimento di Matematica e Informatica "U. Dini" (DIMAI)

MATERIAL SCIENCE, MATHEMATICS

This work contributes to the development of software based tools for high school math teaching, by addressing some questions related to the potential use of Tarski's Foundations of Geometry in Coq. In particular, we first analyze some logical and pedagogical issues of such a possible use; in the second and main part of this work we propose a near-constructive version of Tarski's geometry which is argued to be more natural and more suitable in a teaching environment; finally, we complete Tarski's axiom system for such a purpose by introducing an intuitive axiomatization for the circle. A pedagogical proposal based on cognitive maps and problem-solving is elaborated at the end.

Talk

Ciclo XXVIII

Just a flexible linker? The structural and dynamic
properties of CBP-ID4 as revealed by NMR
spectroscopy

Alessandro Piai

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SPECTROSCOPY, RECOMBINANT PROTEINS

We provide the first structural and dynamic description at atomic resolution of CBP-ID4, the fourth intrinsically disordered linker of the CREB-Binding Protein (CBP). In spite of the mostly disordered nature of CBP-ID4, chemical shifts and relaxation measurements show a significant degree of α -helix sampling in the protein regions enclosing residues 3-25 and 104-128. The data, taken together, also indicate that the two transient α -helices possess different structural properties, being the latter more rigid and stable with respect to the other. An analysis of the amino acid content reveals how prolines play an active role in modulating the structural features of this CBP fragment, promoting disorder along all the polypeptide chain except at the two α -helices locations. The present work opens new insights to a deeper comprehension of the functions of this protein linker, which may exploit its structural and dynamic heterogeneity to modulate the reciprocal orientations of neighboring CBP folded domains and fine tune interaction processes.

Talk

Ciclo XXIX

Study of the conformational changes occurring in human transthyretin that are necessary for amyloid fibril formation in disease and for its role as a detoxifier

Seyyed Abolghasem Ghadami

DOTTORATO IN SCIENZE BIOMEDICHE - Biochimica e Biologia Applicata -
Dipartimento di Scienze Biomediche, Sperimentali e Cliniche

BIOPHYSICS, CELLULAR BIOLOGY, AMYLOID AGGREGATION

Transthyretin is a homotetrameric protein with a total molecular mass of 55 kDa that is one of 30 human proteins associated with systemic amyloidoses. In spite of its link to human pathology, an anti-amyloidogenic effect that prevents fibril formation of the amyloid β peptide associated with Alzheimer's disease has been proposed for TTR. In the light of the results obtained so far, one can hypothesize that TTR may act as an endogenous detoxifier of protein oligomers with potential pathological effects, to inhibiting amyloid fibril formation. In addition, previous data do not offer any insight into the mechanism by which TTR inhibits oligomer toxicity and on the TTR form responsible for such an effect. In this thesis, I will try to address both aspects. I will label TTR with a coumarin derivative, which generates the FRET phenomenon with the endogenous tryptophan residues present in native TTR. The ability of TTR to form soluble oligomers and insoluble fibrils, on the one hand, on to act as a molecular detoxifier, on the other hand, are based on the structural plasticity of the protein and thus on subtle conformational changes in the soluble state of TTR. Finally, we will examine the effects of TTR on the toxicity of extracellularly added oligomers formed by three different proteins, and thus the effects of the TTR-oligomer interaction.

Talk

Ciclo XXIX

Understanding the molecular mechanism of the maturation of cytosolic Iron-Sulfur cluster proteins

Riccardo Muzzioli

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

INORGANIC CHEMISTRY, CELLULAR BIOLOGY, RECOMBINANT PROTEINS

In eukaryotes, both cytosolic and mitochondrial monothiol glutaredoxin proteins bind [2Fe-2S] clusters in the same way, via the formation of a [2Fe-2S]-bridged homodimer. However, while the molecular function of mitochondrial monothiol glutaredoxins has been demonstrated in the last few years, no experimental evidence of [2Fe-2S] cluster transfer pathways directly involving cytosolic monothiol glutaredoxins has been provided yet. Cytosolic monothiol glutaredoxins have been recently proposed, together with other protein candidates, to be implicated in intracellular iron trafficking and sensing, by mediating cytosolic iron trafficking from a hypothetical labile iron pool to iron-dependent enzymes and cell organelles, and by transferring, once they enter the nucleus, a [2Fe-2S] cluster to the iron-responsive transcription factor. Cytosolic monothiol glutaredoxins are implicated in eukaryotes in intracellular iron trafficking and sensing via their bound [2Fe-2S] cluster. Experimental evidences define here a novel role for the human cytosolic monothiol glutaredoxin GRX3 in transferring its [2Fe-2S] clusters to anamorsin, a cytosolic, [2Fe-2S]-binding protein partner. Specific protein recognition between the N-terminal domains of the two proteins is a fundamental prerequisite to drive the [2Fe-2S] cluster transfer from GRX3 to anamorsin.

Talk

Ciclo XXIX

[2Fe-2S] BolA3-GLRX5: a novel player in ISC assembly machinery

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Risonanze Magnetiche (CERM)

SPECTROSCOPY, CELLULAR BIOLOGY

The Iron-Sulfur Cluster assembly machinery located in mitochondria is responsible of the maturation of both mitochondrial and cytosolic iron-sulfur (FeS) proteins. [2Fe-2S] clusters are synthesized in mitochondria on a scaffold protein. Next monothiol glutaredoxin 5 (GLRX5) mediates the transfer of [2Fe-2S] clusters from the scaffold protein to several target proteins. In this frame, BolA-like proteins, which are grouped into three functionally divergent sub-families BolA1-, BolA2-, and BolA3-like proteins, have recently emerged as novel players. It can be postulated that BolA3 functions with GLRX5 in inserting FeS clusters into target proteins. Here, we determined the 3D structure of human BolA3 by NMR. The ^1H - ^{15}N HSQC spectra of apo BolA3 showed well-spread resonances, indicating a well-folded protein. Heteronuclear NMR relaxation measurements were performed to obtain information about protein dynamics. It results that BolA3 is monomeric in solution. After *in vitro* FeS cluster assembly, BolA3 is not able to bind any FeS cluster. Protein-protein interaction between BolA3 and [2Fe-2S] GLRX5 was investigated by NMR titrations. These data showed that two proteins interact forming a stable [2Fe-2S] complex. To define the FeS cluster ligands of BolA3 in the BolA3-GLRX5 complex, C33A and H70A mutants of BolA3 were characterized by NMR and UV-vis spectroscopy.

Talk

Ciclo XXIX

Structural and morphological investigation of TDP-43 aggregates

Claudia Capitini

DOTTORATO IN SCIENZE BIOMEDICHE - Biochimica e Biologia Applicata -
Dipartimento di Scienze Biomediche, Sperimentali e Cliniche

SPECTROSCOPY, BIOPHYSICS, NEURODEGENERATION

Accumulation of intracellular inclusions of TDP-43 in the central nervous system represents the major hallmark correlated to ALS and FTLTDP. Such inclusions have variably been described as amorphous aggregates or more structured deposits. In order to elucidate this point, I utilized two different strategies to produce TDP-43 aggregates: in one case I obtained aggregates *in vitro* from pure C-terminal TDP-43, whereas as a second strategy, I overexpressed TDP-43 in *E. coli* and purified the resulting full-length and C-terminal TDP-43 containing inclusion bodies (IBs). I show that C-terminal aggregates formed *in vitro* are fibrillar, do not contain cross- β structure and do not bind Congo red, but bind thioflavin T depending on conditions. With the second strategy I show that TDP-43 aggregates contained in bacterial IBs do not bind amyloid dyes, possess a disordered secondary structure and are susceptible to proteinase K digestion, thus possessing none of the hallmarks for amyloid. These data reveal an inherently propensity of TDP-43 to form amorphous aggregates, or at most fibrillar structures without an amyloid-like fold. Moreover, these data reproduce all the characteristics found in patients, indicating the usefulness of the two models for understanding the structural and morphological properties of the pathological TDP-43 aggregates.

Talk

Ciclo XXIX

Dissecting brain architecture with a new clearing method

Antonino Paolo Di Giovanna

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Laboratorio Europeo di Spettroscopie non Lineari (LENS)

MICROSCOPY, NEUROSCIENCE

An extensive comprehension of brain architecture is necessary to figure out how the brain works. Therefore, intensive research works are currently ongoing to characterize the complex network of neuronal connections. Optical methods offer the possibility to obtain high-resolution images of biological specimens, nevertheless, investigations deep inside tissues or intact organs is hindered by light scattering. To avoid scattering, biological samples have to be treated in order to make them optically transparent, by means of so-called “clearing methods”. Increasing number of different approaches have been proposed, however each of them presents non-negligible drawbacks, such as structure alteration, fluorescence quenching, incompatibility with immunostaining, long incubation time. We have recently proposed a versatile, simple, rapid and inexpensive method based on a water-soluble agent, 2,2'-thiodiethanol (TDE). We demonstrated the effectiveness of this method applying it on differently processed brain samples and in combination with different optical techniques. Using TDE we were able to obtain a complete reconstruction of a whole mouse hippocampus with serial two-photon tomography and of an entire mouse brain with light sheet microscopy in combination with CLARITY. Furthermore, the method was applied for imaging of human brain tissue from a hemimegalencephaly patient, validating its usefulness in translational research.

Talk

Ciclo XXIX

Evaluation of secretases activity in Alzheimer's disease with fluorescent probes

Niccolò Parenti

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non Lineari (LENS)

MICROSCOPY, NEUROSCIENCE, CELLULAR BIOLOGY

Alzheimer's disease is a chronic neurodegenerative pathology that is characterized by the loss of memory and other cognitive functions, and whose causes are still poorly understood. One of the hypothesis is the involvement of the β -amyloid peptide, which is generated after the cleavage of APP (Amyloid Peptide Precursor) by specific secretases and polymerizes to form toxic aggregates. Previous studies demonstrated a link between Alzheimer and cholesterolemia, so our purpose is to evaluate the activity of the secretases and their interactions with the APP in different conditions of cholesterol levels. Using genetic engineering techniques, we produced several constructs of APP and secretases (α , β , γ) fused with different fluorescent proteins. We fused APP with two fluorescent protein, GFP at the C-term and mCherry at the N-term. In this manner we obtained a fusion protein with both sides (intra- and extra-cellular) marked. To estimate the activity of the secretases we used the red/green ratio of fluorescent signal from cells in which we varied the expression level of the secretases.

Talk

Ciclo XXX

Oleuropein aglycone in the TgCRND8 mouse model of A β deposition

Pamela Nardiello

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Dipartimento di Scienze Biomediche, Sperimentali e Cliniche

PHARMACOLOGY, NEUROSCIENCE, BIOCHEMICAL

Alzheimer's disease (AD) is an age-related disorder characterized by increased accumulation of intracellular neurofibrillary tangles (NFTs) and extracellular amyloid- β (A β deposits and A β deposition is considered the causative event of AD pathology. Environmental and lifestyle factors play a role in the risk of developing AD and adherence to the MD has been demonstrated to be beneficial for AD and cognitive performance. We report that 8 weeks dietary supplementation of oleuropein aglycone (OLE) (50 mg per kg of diet and 12.5 mg per kg of diet), the major phenol present in extra virgin olive oil, significantly reduces *de novo* β deposition and favors preformed plaque disassembly in the TgCRND8 mouse model of A β deposition at different stages of the pathology (3, 6 and 12 months of age). The treatment strongly improves the cognitive performances of young/middle age TgCRND8 mice respect to un-supplemented diet and counteracts the aggregation process of A β . Interestingly OLE-fed TgCRND8 mice show a significant reduction of A β 3pE-42 load, both as total plaque area and plaque number, in somatosensory/parietal and piriform/entorhinal cortices and hippocampus. These studies suggest that dietary supplementation with OLE may prevent/delay the occurrence of AD and reduce the severity of its symptoms.

Talk

Ciclo XXVIII

miRNA in Amyotrophic Lateral Sclerosis: pathogenic role and potential biomarkers

Michele Benigni

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NEUROSCIENCE, CELLULAR BIOLOGY

Amyotrophic lateral sclerosis (ALS) is an untreatable, fatal neuromuscular disease caused by degeneration of motor neurons and characterized by progressive wasting and weakness of limbs, bulbar and respiratory muscles symptoms. Accumulating evidence indicates that various microRNAs (miRNAs), expressed in the brain, play a key role both in physiological and pathological conditions, particularly in neurodegenerations. The present project consists in the research of specific miRNAs characterizing the ALS patients. MiRNAs in cerebrospinal fluid (CSF) of 16 patients with ALS and 16 healthy controls have been analysed by Real-Time PCR. A panel of the 372 most abundantly expressed and best-characterized miRNAs have been analysed by miRNA profiling. This analysis has revealed differentially expressed miRNAs in CSF from ALS patients compared to controls and a cluster of 14 molecules has been selected for the validation experiments. Among those, three miRNAs resulted upregulated in patients compare to controls and eleven downregulated. By further analysis miR195-5p, miR21-5p and miR-148a-3p showed significantly lower expression in ALS patients and two miRNAs (let7f-5p and miR15b-5p) resulted downregulated and close to borderline significance. The downregulation of those miRNAs has not been previously described in other neurodegenerative diseases and seems to be a distinctive signature of ALS.

Talk

Ciclo XXX

Molecular and genetic analysis of OPA1, CAPN3 and DYSF gene

Sara Aguti

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NEUROSCIENCE, CELLULAR BIOLOGY, GENETICS

Autosomal Dominant Optic Atrophy (ADOA) is the most prevalent hereditary optic neuropathy typically presenting with a slowly progressive, painless, bilateral visual loss. The main ADOA-causing gene is the nuclear OPA1 gene, which encodes a mitochondrial GT-Pase involved in the mitochondrial fusion, cristae organization and control of apoptosis. During my PhD, I have to analyze patients with suspected ADOA for OPA1 mutations, to nowadays we found 3 new mutations in approximately 30 patients. In order to understand the possible pathogenic role of mutations not yet described, has been analyzed the mRNA sequence and has been performed an *in silico* analysis. In addition, I'm carrying on the work of my MSc thesis. During my thesis I have analyzed in approximately 60 patients with suspected Limb-Girdle Muscular Dystrophy (LGMD), an autosomal recessive muscle disease characterized by progressive atrophy and weakness of the proximal limb muscles. First of all we set up molecular diagnosis of LGMD2A caused by mutations in CAPN3 gene, the predominant form of LGMD2. We found six patients with CAPN3 mutations, two of which novel. Subsequently we set up molecular diagnosis of LGMD2B, caused by mutations in DYSF gene, since it represents the second most frequent form of LGMD2.

Talk

Ciclo XXVIII

Single-molecule study for a graphene-based nano-position sensor

Giacomo Mazzamuto

INTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS -
Laboratorio Europeo di Spettroscopie non Lineari (LENS)

MATERIAL SCIENCE, MICROSCOPY, SPECTROSCOPY, OPTICS AND PHOTONICS

In this study we lay the groundwork for a graphene-based fundamental ruler at the nanoscale. It relies on the efficient energy-transfer mechanism between single quantum emitters and low-doped graphene monolayers. Our experiments, conducted with dibenzoterylene (DBT) molecules, allow going beyond ensemble analysis due to the emitter photo-stability and brightness. A quantitative characterization of the fluorescence decayrate modification is presented and compared to a simple model, showing agreement with the d^{-4} dependence, a genuine manifestation of a dipole interacting with a 2D material. With DBT molecules, we can estimate a potential uncertainty in position measurements as low as 5 nm in the range below 30 nm.

Talk

Ciclo XXIX

Raman measurements of hydrogen clathrate hydrate synthesized from liquid

Leonardo del Rosso

DOTTORATO IN FISICA E ASTRONOMIA - Fisica - Consiglio Nazionale delle Ricerche
(CNR)

PHYSICAL CHEMISTRY-CHEMICAL PHYSICS, SPECTROSCOPY, MATTER PHYSICS

The nucleation and growth from the liquid phase of a solid clathrate-hydrate is a process even less understood and more difficult to study compared to that of a pure liquid. By means of *in situ* Raman spectroscopy, we have examined this phenomenon for the system hydrogen and water. Our sample is initially a liquid solution of hydrogen in water in contact with pressurized hydrogen gas at 2 kbar and at a temperature of 264 K (i.e. outside the stability region of common ice). After about 10 hours, we start to detect the vibrational spectrum of caged hydrogen molecules which increases in intensity while the solid clathrate grows. From the analysis of the Raman intensity, we can infer the population of the small (5^{12}) and large ($5^{12}6^4$) cages as a function of time during the hydrogen clathrate growth. Its behaviour, observed here for the first time, has some analogies with what observed in the more studied case of methane hydrate, where the small cages play a key role in the first stage of nucleation. However the possibility for hydrogen of multiple occupation of the large cages introduces an extra degree of freedom for the determination of the hydrate stoichiometry.

Talk

Ciclo XXIX

Universal state orthogonalizer and qubit generator

Luca Costanzo

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Laboratorio Europeo di Spettroscopie non Lineari (LENS)
OPTICS AND PHOTONICS, QUANTUM INFORMATION

The fundamental unit in classical information theory is the binary unit or bit. Its counterpart in a quantum framework is the quantum bit (qubit), which, unlike its classical version, can assume at the same time both the orthogonal values allowed, in a so-called quantum superposition.

I present an experimental demonstration of an universal strategy for producing a quantum state that is orthogonal to an arbitrary pure input one, even if only a very limited amount of information about the latter is available. Arbitrary quantum superpositions of the two mutually orthogonal states (a qubit) are then produced by a simple change in the experimental parameters. This scheme works equally well for arbitrary input fields and, since it is a universal procedure, may prove an important building block for quantum state engineering and quantum information processing with continuous-variable qubits.

Talk

Ciclo XXX

Can a superfluid in one dimension flow without dissipation?

Simona Scaffidi Abbate

DOTTORATO IN FISICA E ASTRONOMIA - Fisica - Dipartimento di Fisica e Astronomia

THEORETICAL PHYSICS, OPTICS AND PHOTONICS, MATTER PHYSICS, ATOMIC PHYSICS, APPLIED PHYSICS

A Bose-Einstein condensate is a system where quantum effects operate on a macroscopic scale. It is a state of matter close to $T = 0$ where a macroscopic number of particles stays in the lowest quantum energy level. If the particles interact, quantum effects lead to the ability to sustain a particle current at constant velocity without dissipation, even in presence of an obstacle. In other words, a Bose-Einstein condensate is a superfluid. If a superfluid is confined in one spatial dimension, quantum effects can destroy superfluidity. Indeed, quantum fluctuations arising from the interactions between particles lead to the so-called quantum phase-slips, that produce strong fluctuations in the phase of the superfluid. These fluctuations are observed as a dissipation of energy in the system, which stops to behave as a superfluid even if the temperature is zero. Quantum phase-slips have so far been observed only in selected solid-state systems. We have now performed an experiment with a gas of ultracold atoms that demonstrates the presence of quantum phase-slips also in atomic superfluids. This result is important because Bose-Einstein condensates are very well controllable, and one can think of studying fundamental aspects of quantum phase-slips that have not yet been understood.

Talk

Ciclo XXVIII

3D Anderson localization with ultracold atoms

Giulia Semeghini

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Laboratorio Europeo di Spettroscopia non Lineari (LENS)

MATTER PHYSICS, ATOMIC PHYSICS

When traveling through a disordered environment, quantum particles may exhibit a localization phenomenon arising from interference effects between multiple scattered waves. This is the well-known Anderson localization (AL), discovered more than 50 years ago and still at the heart of intense research. The initial context of its formulation and study was solid state physics, since AL was found to be relevant in the occurrence of metal-insulator transitions. It was later discovered that the phenomenon is extremely general, since it affects every kind of waves in a disordered medium, ranging from classical waves to quantum wavefunctions. This allowed to study AL in many other physical systems that were easier to manipulate and study than metallic samples. Ultracold atomic systems now offer the possibility of an unprecedented control on all the relevant parameters of the system, from the shape and intensity of the potential to the energy and interactions in the atomic sample. In our experiment we use a Bose-Einstein condensate of potassium-39 atoms to investigate the occurrence of AL in three spatial dimensions. We study in particular the occurrence of the quantum phase transition occurring when the atoms enter the localization regime.

Talk

Ciclo XXX

QCL-based metrological-grade THz spectroscopy tools

Annamaria Campa

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Dipartimento di Fisica e Astronomia
SPECTROSCOPY, MATTER PHYSICS

The Terahertz region of the electromagnetic spectrum covers a still under-explored gap, though having potential not only for countless applications in strategic fields, like bio-medical diagnostics, communication technology, security and defense, but also for a number of studies on molecules, since rotational transitions generally fall in the far-infrared range. These transitions typically have large line-strengths, and can be very suitable not only for the development of high-sensitivity trace-gas sensing techniques, but also for investigating fundamental aspects in molecular physics. High precision THz molecular spectroscopy therefore promises amazing scientific and technological applications, provided that sources with suitable high power, wide tunability and narrow linewidth, such THz Quantum Cascade Lasers are available. The first application of a QCL phase-locked to a free-standing THz Frequency Comb Synthesizer (FCS) was recently demonstrated, achieving a state-of-the-art accuracy of 4×10^{-9} in the determination of the absolute frequency of a THz transition. Saturated-absorption spectroscopy, and the possibility to use well-established spectroscopic tools, such as cavity resonators, are the natural evolution of experimental setups aiming to overcome the limitation set by the Doppler broadening of molecular lines at room temperature, paving the way to next generation THz metrological tools.

Talk

Ciclo XXVIII

Coevolution Black Holes and host galaxies

Stefano CarnianiDOTTORATO IN FISICA E ASTRONOMIA - Astronomia - Dipartimento di Fisica e
Astronomia

SPECTROSCOPY, MATTER PHYSICS

One of the most important astronomical discoveries in the last 20 years is that most local massive galaxies host a supermassive Black Hole in their centre. The most relevant discovery supporting the evidence of a connection between the BH and its host galaxy is the tight correlation between the BH mass and the mass and luminosity of the stars in nuclear region of the galaxy. These relations led to believe that BHs and galaxies co-evolve by regulating each other's growth. So far, the reason why a connection between these two classes of objects exists is still unclear. An important factor is the impact that the energy realized by BH accretion has on the surrounding gas. A growing BH releases plenty of energy in the galaxy expelling gas at large scale and quenching star formation activity. Galactic-scale outflows are one of the major feedback mechanisms regulating the growth of galaxies. Despite the important role outflows play in galaxy evolution, the occurrence and properties of outflows are not well constrained yet. By taking advantage of the integral field spectroscopy technique we can unambiguously identify wind galaxies by investigating the emission line kinematics. These observations suggests a clear evidence of feedback.

Talk

Ciclo XXIX

Dy(LH)₃dmf complex: a multitechnique approach for a meaningful magnetic characterisation

Eva Lucaccini

DOTTORATO IN INGEGNERIA INDUSTRIALE - Scienza ed Ingegneria dei Materiali -
Dipartimento di Chimica "Ugo Schiff"

INORGANIC CHEMISTRY, MATERIAL SCIENCE, MAGNETISM

We present here an overview of the appropriate procedures needed to characterise the magnetic behaviour of Lanthanide based molecular samples, focusing on some results about Dy(LH)₃dmf complex. The compound, both pure and doped in the Yttrium(III) analogue, was analysed by powder XRD evidencing that the crystalline phase was consistent with the one determined by single crystal diffraction. The static magnetic properties of the sample excluded strong interaction among neighbouring paramagnetic centres but suggested the presence of non magnetic residuals that could not be observed in powder XRD. We then performed an investigation on the magnetization dynamics of the complex, studying its response when an oscillating magnetic field is applied. We found that the complex exhibited a non-zero imaginary susceptibility, meaning that its magnetization relaxes slowly, both in zero and non-zero magnetic static field. The magnetic anisotropy of the complex was finally investigated by means of Electron Paramagnetic Resonance (EPR) and Torque Magnetometry. In this case the EPR signal was absent, probably due to the state composition of the ground doublet, while Torque measurements evidenced the presence of an easy axis of magnetization, of orientation and degree of axiality comparable to those predicted using *ab initio* calculations.

Talk

Ciclo XXIX

Assembling Fe₄ Single Molecule Magnets: paving the way to molecular spintronics

Irene Cimatti

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

INORGANIC CHEMISTRY, MATERIAL SCIENCE, SURFACE SCIENCE, PHYSICAL
CHEMISTRY-CHEMICAL PHYSICS

Single Molecule Magnets (SMMs) have intriguing properties which make them possibly suitable for applications in molecular spintronics devices. The interface between the different layers in such systems seems to play a fundamental role and it is key to understand their behaviour. For this reason the inspection of the very first layer in contact with the substrate is of crucial importance.

After deposition, the peculiar magnetic properties of complex molecules such as SMMs tend to vanish. The choice of the molecule to use is therefore important. One of the most promising family of SMMs is Fe₄: some conveniently functionalised clusters can be deposited as Self-Assembled Monolayers while other molecules of this family can be sublimated on the surface.

A precise characterisation of the deposited layer at monolayer and submonolayer coverage requires several surface sensitive techniques. In this study we sublime an Fe₄ cluster on metallic surfaces and characterise the deposited layer by Scanning Tunneling Microscopy and X-rays Photoelectron Spectroscopy to probe the integrity of the molecules and finally by X-rays Magnetic Photoelectron Spectroscopy to measure their magnetic properties.

Talk

Ciclo XXVIII

Exchange bias in $\text{Co}_x\text{Fe}_{1-x}\text{O}(\text{AFM})|\text{Co}_x\text{Fe}_{3-x}\text{O}_4(\text{FiM})$
Core|Shell nanoparticles

Elisabetta Lottini

DOTTORATO IN INGEGNERIA INDUSTRIALE - Scienza ed Ingegneria dei Materiali -
Dipartimento di Chimica "Ugo Schiff"

INORGANIC CHEMISTRY, MATERIAL SCIENCE, MAGNETISM

The exchange bias effect manifests as a horizontal hysteresis loop shift and coercivity increase due exchange coupling at the interface between two different magnetically ordered phases. Interestingly, being an interface effect, exchange bias is only observed at the nanoscale. Here, an investigation on inverted antiferromagnetic(AFM)|ferrimagnetic(FiM) core|shell nanoparticles of formula $\text{Co}_x\text{Fe}_{1-x}\text{O}|\text{Co}_x\text{Fe}_{3-x}\text{O}_4$, is presented. Narrowly size distributed core|shell nanoparticles with mean diameter from 6 to 18 nm have been synthesized by thermal decomposition of mixed iron(III) and cobalt(II) metal-oleate, leading to the formation of an AFM-core ($\text{Co}_x\text{Fe}_{1-x}\text{O}$) which is passivated under air yielding the corresponding FiM-shell ($\text{Co}_x\text{Fe}_{3-x}\text{O}_4$). Interestingly, all the samples are characterized by the presence of a constant FiM shell thickness ($t_{\text{shell}} = 2$ nm) and a variable AFM core diameter ($d_{\text{core}} = 2, 5, 11$ and 14 nm). Low temperature hysteresis loops reveal the presence of exchange bias and increased coercivities as expected for a good exchange coupling between core and shell phases. Since the exchange bias effect is affected in an entangled way by the core and shell size, the synthesized NPs have been used to systematically address the effect of the size of AFM counterpart, which has been less studied than the FiM size dependent properties.

Talk

Ciclo XXVIII

Mapping the spin structure of a chiral magnet

Mauro Perfetti

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

PHYSICAL CHEMISTRY-CHEMICAL PHYSICS, MATTER PHYSICS, MOLECULAR
MAGNETISM

Chirality is an important property of many molecules, including some relevant compounds the evolution of life. If a magnetic molecule is fashioned in a chiral structure, both the time reversal and the space inversion symmetry are simultaneously broken. Moreover magnets characterized by a chiral crystallographic structure exhibit a chiral spin structure that origins novel magneto-optical phenomena such as the magneto-chiral dichroism and the non-linear magneto optical effect. It is thus important to precisely know the spin orientation of the magnetic ions in chiral molecules, however this is not an easy task because it requires synchrotron light. To overcome this limitation, we used a combination of a simple but powerful technique (cantilever torque magnetometry) and the unique magnetic properties of the lanthanide ions. The studied chiral compound was an helix of six Dy atoms connected by organic ligands. The extreme sensitivity of cantilever torque magnetometry, flanked by an accurate home-made fitting program, allowed to map the entire spin structure of the single centres performing only two orthogonal rotations.

Talk

Ciclo XXVIII

Mo and stable U isotopes as tracers for subduction
components in the Quaternary West-Mediterranean
potassic and ultrapotassic magmatism

Martina Casalini

DOTTORATO IN SCIENZE DELLA TERRA - Dipartimento di Scienze della Terra (DST)

GEOCHEMISTRY AND VOLCANOLOGY, MINERALOGY AND PETROLOGY

The central-western Mediterranean is one of the most important areas on Earth for studying subduction-related potassic and ultrapotassic magmatism. In a very restricted area where rocks with different chemical composition and geochemical features occur. These rocks invariably show the highest levels of incompatible trace elements ever seen in any volcanic arc. These features are thought to be derived through the recycling of sediments via subduction within the mantle wedge, and their extreme trace element enrichments make them unique for understanding the roles of different subduction-related metasomatic agents (e.g. fluid vs melt). We propose to investigate this issue considering two stable isotopic systematics that are notably fractionated by redox-related processes as those occurring between seawater and oceanic sediments. We measured Mo and stable U isotopes, with the high-resolution MC-ICP-MS using a double-spike technique, on selected volcanic rocks from four Italian magmatic provinces and representative samples of subducting sediments. We have interpreted our results to recognize U and Mo isotopic signature of sediments, with different lithology and chemical composition, recorded into the selected volcanic rocks, and to set new constraints on the metasomatic agents responsible for the transition from silica oversaturated lamproite-like to strongly silica undersaturated HKS magmas.

Talk

Ciclo XXX

A simplified procedure to assess 1D seismic response in Tuscany Region

Giacomo Peruzzi

DOTTORATO IN SCIENZE DELLA TERRA - Dipartimento di Scienze Fisiche, della Terra
e dell'Ambiente (Università di Siena)

NATURAL HAZARDS, GEOPHYSICS

In the “Indirizzi e Criteri per la Microzonazione Sismica” Italian regions are suggested to realize abacuses to assess 1D seismic response in microzoning studies. Abacuses are used to estimate seismic amplification in “stable areas characterized by amplification of the ground motion due to the local litho-stratigraphic or morphological configuration” in which it is possible to use a simplified approach. In practice these abacuses are tables which contain values of the amplification factor (FA) which describe seismic amplification of every Tuscan litho-stratigraphic configuration, compared with a reference one. Their realization starts with collecting and classifying by homogeneous types the great amount of geological, geotechnical and seismological data (from Tuscany Region database). This information is used to randomly generate a lot of “simulated” stratigraphic and seismic profiles, from which FA values are calculated. FA values distribution is then statistically characterized, using parameters which are able to define each litho-stratigraphic configuration. This kind of procedure has the aim to appraise the geological Tuscan database and to give a easy and useful tool for every professionals who works in the field of seismic microzonation.

Talk

Ciclo XXX

Preliminary studies of GV7, a new drilling site in East Antarctica

Laura Caiazzo

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

ANALYTICAL CHEMISTRY, ENVIRONMENTAL / POLLUTION

In the framework of the new project: 'The IPICS 2k Array: a network of ice core climate and climate forcing records for the last two millennia', born within the International Partnerships in Ice Core Sciences (IPICS), a 265 m deep ice core was retrieved in a new drilling site, GV7 (70°41'S - 158°51'E) in East Antarctica. This site is characterized by a relatively high snow accumulation (about 240 mm water eq.), allowing a better understanding of the climatic variability in the last 2000 years. The aim of this work is to present the chemical stratigraphy of the chemical markers coming from a snow pit, in order to carry out a preliminary survey of their preservation and temporal patterns at this site. Samples were collected during 2013/14 field season and analysed in Italy by Ion Chromatography for main and trace anions and cations. Basing on the seasonal trends of selected climatic and environmental proxies (such as non-sea-salt sulphate, methanesulphonic acid and nitrate), an accurate dating of this snow pit is being performed and will be basic for the interpretation of the achieved records and for their comparison with records from snow pits or ice/firn cores collected at different sites.

Talk

Ciclo XXVIII

Energy, hydrogen and chemicals by renewable alcohols electrooxidation

Marco Bellini

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Consiglio Nazionale delle Ricerche (CNR)

INORGANIC CHEMISTRY, MATERIAL SCIENCE, ENVIRONMENTAL / POLLUTION, ENERGY ENGINEERING, ELECTROCHEMISTRY

Selective production of chemicals from renewable resources with contemporaneous release of energy is one of the most desired targets of sustainable chemistry. Direct Alcohols Fuel Cells (DAFCs) operating in alkaline environment are the only devices that can achieve this objective: DAFCs produce electricity oxidizing at low temperatures renewable alcohols like ethanol or glycerol to their respective carboxylic compounds. These products have a high added value due to their use as raw chemicals for fine chemical industry. The anodic electrocatalyst has a crucial role in this selective electrooxidation. Palladium nanoparticles based electrocatalysts represents the the state of the art of the anodic electrocatalyst for DAFCs. Unfortunately this kind of catalysts can selectively oxidize ethanol to acetate but they fail in polyalcohols selctive oxidation. The employment of a rhodium complex based electrocatalyst can solve this problem, in addition it allows to reduce the preciuos metals loading in these anodic electrocatalyst because each metal center is active for electrocataklysis. The use of oraganometallic anodic electrocatalysts can be transferred to alkaline alcohols reformers, electrolisers that produce hydrogen with a 60 % lower energy consumption respect traditional water electrolyzers due to the replacment of the anodic oxygen evolotuion reaction whith an alcohol oxidation process.

Talk

Ciclo XXX

Investigation of the structural properties of MgO-based eco-sustainable cements

Monica Tonelli

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

MATERIAL SCIENCE, PHYSICAL CHEMISTRY-CHEMICAL PHYSICS

Cement formulations based on reactive periclase (MgO) constitute one of the most promising emerging technologies toward eco-sustainable binders, with reduced CO₂ emissions as compared to the traditional CaO-based cements. In the presence of water, the MgO/silicate mixtures hydrates and forms a binder phase, M-S-H (magnesium silicate hydrate), a colloidal gel analogue to hydrated calcium silicate hydrate, C-S-H, present in traditional cements. A detailed knowledge of these cements is still lacking and foreclose its use. The aim of this research is to provide a systematic investigation of these new formulations, to unravel the relationship among composition, structure and properties. In this work, the effect of mixing traditional cement and MgO-based eco-sustainable cement were evaluated. The hydration kinetics of MgO/silicate mixtures were investigated by means of differential scanning calorimetry, since controlling the kinetics of the hydration reaction is a technologically important target especially for practical applications. Concurrently, pastes were characterized starting from the molecular level up to the micro/macroscopic scale using a multi-scale approach based on many techniques (DTG, FTIR, XRD, BET, SEM/EDX, SS-NMR, SAXS).

Talk

Ciclo XXVIII

Good vibrations: the role of substrate-borne vibrations
in mating behaviour of the leafhopper *Empoasca vitis*

Rachele Nieri

DOTTORATO IN BIOLOGIA - Etologia ed Ecologia - Dipartimento di Biologia (BIO)

ECOLOGY / ETHOLOGY / EVOLUTION

Substrate-borne vibrational signals are widespread in many insect taxa. In some species of *Hemiptera* they are the main channel of communication during mating behavior, mediating the identification and location of partners. The leafhopper *Empoasca vitis* is a grapevine pest, despite its economic importance, to date the mating behavior and associated vibrational communication of this species are still undescribed. For the first time in the present study, by means of laser vibrometer and behavioral observations, we investigated the mating behavior of *E. vitis*, describing the role of substrate-borne vibrational signals in pair formation and the mating activity throughout the day. Pair formation begins with male's call (MC), which consists of a complex signal. If the female is present, she replies to MC and a duet is maintained until the copula occurs. Even if males call throughout the day, the number of matings is lower during the night in darkness, suggesting visual stimuli to play a role at least in the last part of mate location. The knowledge acquired thanks to this work may contribute to the development of a synthetic signal able to interfere with the mating behavior of the species.

Talk

Ciclo XXIX

Copulatory success in lekking fallow (*Dama dama*)
bucks: hypotheses testing using generalized structural
equation models

Sonia Lombardi

DOTTORATO IN BIOLOGIA - Etologia ed Ecologia - Dipartimento di Biologia (BIO)

ECOLOGY / ETHOLOGY / EVOLUTION, STATISTICAL ANALYSIS

We studied the causal factors explaining the differences in copulatory success among lekking fallow bucks, using Generalized Structural Equation Models (GSEM). Data have been collected in the population of fallow deer of the Preserve of Castelporziano (Rome, Italy) during the rut within the lekking area. Bucks were taped and after individually identified. Morphological and Fluctuating Asymmetry measures were obtained from the antlers. We recorded for each buck its position, the number of fights, its sexual activity, the number of females and fawns inside the Lek. A total of 11 behavioural variables (dominance, reproductive success, harem size, lek attendance) were used in the statistical analysis. The most studied lekking deer show a strong evidence for female mate choice. Nevertheless dominance rank is correlated to male reproductive success. We developed two *a priori* models to test two principal hypothesis: female choice in which we assumed that females preferred a male for its good genes; male dominance in which we assumed that copulatory success is depending on dominance rank. We used the AIC to select the model with other fitting index. Model comparison and analysis of the models' fitting showed that the female choice model explain better the observed covariance patterns.

Talk

Ciclo XXVIII

Qualification and traceability of Tuscany milk through NMR-based metabolomics

Claudio Santucci

INTERNATIONAL DOCTORATE IN STRUCTURAL BIOLOGY - Centro di Ricerca di
Risonanze Magnetiche (CERM)

AGRIFOOD, METABOLOMICS

Commercial value of dairy products is associated with origin and composition of milk, so information about quality and traceability are necessary. We used $^1\text{H-NMR}$ spectroscopy to profile different types of milk samples: raw milk samples coming from 10 stables in Tuscany, collected in two different periods; supermarket milk collected in three distinct periods and organic and non-organic milk. Results show that through metabolic profile is possible to distinguish samples from their belonging stables, although seasonal variability is present. Analyzing feeding rations, we found three different nutritional patterns that are well-separated in the metabolic profiles plot. Results show that milk metabolic profiles are strongly influenced by cow nutrition. The most important difference was between stables fed with silages and not, further, from the analysis of metabolites content we observed a 3-fold decreasing of lecithin in stables not fed with silages. We correlated also spectral data and nutritional data to understand relations between feeding and metabolites. In this study we have demonstrated that $^1\text{H-NMR}$ spectroscopy can be an accurate tool to analyze milk and to obtain information about traceability; furthermore, it is possible to extract information about feeding of cows, a very important issue to assess the quality of dairy products.

Talk

Ciclo XXVIII

Multivariate analysis of combined first-derivative
micro-Raman and reflectance FT-NIR spectra for the
analysis of binder materials both neat and in simulated
mixtures

Serena Carlesi

DOTTORATO IN SCIENZE CHIMICHE - Scienza della Conservazione dei Beni Culturali -
Dipartimento di Chimica "Ugo Schiff"

CULTURAL HERITAGE PRESERVATION, SPECTROSCOPY

A systematic study concerning the potential of applying the multivariate technique Principal Component Analysis (PCA) on combined first derivative micro-Raman and reflectance FT-NIR spectra to study and discriminate different types of binding media both neat and in mixture with pigments is reported. In this work traditional binding media such as drying oils (linseed oil, walnut oil, poppy oil and stand-oil originated from linseed oil), proteinaceous (egg yolk, egg white, whole egg, casein, rabbit skin glue, strong glue and fish glue) and polysaccharides (Arabic gum and Tragacanth gum) were analyzed. Furthermore, a series of paint mixtures, using lead white, zinc white, azurite, synthetic and natural ultramarine, phthalocyanine blue were prepared with linseed oil and poppy-seed oil. Each analyzed sample was individually applied on four microscope glass slides and left to dry on a shelf for nine months before analysis. Micro-Raman and FT-NIR spectroscopies provide a complementary information which can be used to identify the pigments and binders in paint samples. A combination of first derivative micro-Raman and FT-NIR spectra enhances the extraction of vibrational and statistical information from each analyzed sample by means of the use of PCA. Each new combined spectrum is characterized by both fundamental and combination/overtone modes.

Talk

Ciclo XXIX

Conservation and restoration of archaic stones of ancient cities of Euromos and Iasos Turkey

Halit Canol

DOTTORATO IN SCIENZE CHIMICHE - Scienza della Conservazione dei Beni Culturali -
Dipartimento di Chimica "Ugo Schiff"

MATERIAL SCIENCE, POLYMER SCIENCE, MINERALOGY AND PETROLOGY

Scientific methodologies has increased in the field of archaeological conservation and in archaeology is essential to develop the scientific research in material properties; prerequisite for conservation work. The complexity is also related to the fact that the study of marble artefacts from ancient cities of Euromos and Iasos are multidisciplinary activity involving the fields of archaeology, history, art as well as the scientific disciplines of geology, chemistry and physics. Stone samples from the monuments of these ancient cities will be analyzed to determine their organic and inorganic compositions. Researches concern the investigation of the physical, chemical and mechanical characteristics in order to estimate the durability of these pieces of monuments and to select suitable conservative treatments. Tests for the evaluation of efficacy and durability of conservative treatments, in relation to the environmental conditions which the stones are submitted, will be properly identified and realized. *In situ* analyses by thermo camera and protimeter for monitoring temperature and relative humidity on stone surfaces and in the environment will be carried out. Innovative compounds are (mainly those belonging to the partially fluorinated polymers class) for the protection or consolidation of stones will be studied and tested on laboratory as well as *in situ*.

Posters

P – 1. Integrating field survey on geo-environmental factors and orthophoto information to monitor coastal dune habitats – A pilot study to evaluate coastal dune vulnerability

Fernanda Alquini DOTTORATO IN SCIENZE DELLA TERRA

P – 2. Climosequence approach to monitor the effects of exposure and altitude on physical, chemical and microbial properties of alpine soils

Tommaso Bardelli DOTTORATO IN SCIENZE AGRARIE E AMBIENTALI

P – 3. Development of a nonlinear multimodal microscopic platform and its application to the study of arterial tissues

Enrico Baria INTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS

P – 4. Nano- and microcapsules: synthesis and physical chemical characterization.

Arianna Bartolini DOTTORATO IN SCIENZE CHIMICHE - *Chimica*

P – 5. New acridine based ligands for metal ion binding and fluorescence sensing

Francesco Bartoli DOTTORATO IN SCIENZE CHIMICHE -
Chimica

P – 6. Microwave assisted pyrolysis of biomass

Mattia Bartoli DOTTORATO IN SCIENZE CHIMICHE - *Chimica*

P – 7. Novel non-aqueous amine solvents for reversible
CO₂ capture

Francesco Barzagli DOTTORATO IN SCIENZE CHIMICHE -
Chimica

P – 8. Electrodeposition from Ionic Liquids (IL) and
Deep Eutectic Solvents (DES)

Enrico Berretti DOTTORATO IN SCIENZE CHIMICHE - *Chimica*

P – 9. Italian adaptation of the Parental Attitudes
Scales

Giuly Bertoli DOTTORATO IN SCIENZE CLINICHE - *Psicologia e
Terapia del Dolore*

P – 10. 6-aminopyridine-3,5-dicarbonitriles as
non-nucleoside adenosine A1 receptor agonist

Marco Betti DOTTORATO INTERNAZIONALE IN AREA DEL
FARMACO E TRATTAMENTI INNOVATIVI - *Scienze Farmaceutiche*

P – 11. Multi-level Modeling of Lanthanide-containing materials by *ab initio* methods

Matteo Briganti DOTTORATO IN SCIENZE CHIMICHE - *Chimica*

P – 12. QCL-based metrological-grade THz spectroscopy tools

Annamaria Campa INTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS

P – 13. Evaluation of diaphragm thickening by diaphragm ultrasonography: a reproducibility and repeatability study

Iacopo Cappellini DOTTORATO IN SCIENZE CLINICHE - *Scienze Anestesiologiche e Chirurgiche*

P – 14. Fast analysis of glibenclamide and its related substances by capillary electrophoresis

Claudia Caprini DOTTORATO INTERNAZIONALE IN AREA DEL FARMACO E TRATTAMENTI INNOVATIVI - *Scienze Farmaceutiche*

P – 15. Trough territorial complexity: megacity and water uses

Benedetta Caprotti DOTTORATO IN ARCHITETTURA - *Progettazione Urbanistica e Territoriale*

P – 16. 2D-Fluorescence studies of neat binding media and simulated paint mixtures

Serena Carlesi DOTTORATO IN SCIENZE CHIMICHE - *Scienza della Conservazione dei Beni Culturali*

P – 17. Matarka: a new ungrouped iron meteorite from Morocco

Vanni Moggi Cecchi DOTTORATO IN SCIENZE DELLA TERRA

P – 18. Glycosylated natural saponins for autoantibody recognition

Anne-Sophie Champy DOTTORATO IN SCIENZE CHIMICHE - *Chimica*

P – 19. Exploring the genetic basis of symbiotic performance in rhizobia: the *acdS* gene in *Sinorhizobium meliloti*

Alice Checcucci DOTTORATO IN BIOLOGIA - *Genetica e Microbiologia*

P – 20. Synthesis and characterization of new materials for technological and solar devices

Serena Cinotti DOTTORATO IN SCIENZE CHIMICHE - *Chimica*

P – 21. The landscape as an orienting factor in *Talorchestia martensii*

Alice Ciofini DOTTORATO IN BIOLOGIA - *Etologia ed Ecologia*

P – 22. Melanocytic nevi and drugs: results of an observational study

Roberta Colucci DOTTORATO IN SCIENZE BIOMEDICHE - *Oncologia Sperimentale e Clinica*

P – 23. Optical and electrochemical characterization of acridine ligands for sensoristic applications

Luca Conti DOTTORATO IN SCIENZE CHIMICHE - *Chimica*

P – 24. Generation of hybrid entanglement of light

Luca Costanzo INTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS

P – 25. Involvement of central histaminergic system in the oleoylethanolamide-induced antidepressant-like effect in the mouse tail suspension test

Alessia Costa DOTTORATO INTERNAZIONALE IN AREA DEL FARMACO E TRATTAMENTI INNOVATIVI - *Farmacologia, Tossicologia e Trattamenti Innovativi*

P – 26. Aerobic oxidation of hydroxylamines to nitrones catalyzed by a supported gold catalyst

Giampiero D'Adamio DOTTORATO IN SCIENZE CHIMICHE - *Chimica*

P – 27. Raman measurements of hydrogen clathrate hydrate synthesized from liquid

Leonardo del Rosso DOTTORATO IN FISICA E ASTRONOMIA - *Fisica*

P – 28. Multi-target data association using sparse reconstruction

Dario Di Fina DOTTORATO IN INFORMATICA, SISTEMI E TELECOMUNICAZIONI

P – 29. Impairment of cell autophagy in primary CTSF/CLN13 cells

Stefano Doccini DOTTORATO TOSCANO DI NEUROSCIENZE

P – 30. Towards single-atom imaging in a strongly interacting Rydberg gas

Giulia Faraoni DOTTORATO IN FISICA E ASTRONOMIA - *Fisica*

P – 31. Biotin-decorated carbon nanotubes as drug carrier to increase effect of doxorubicin against breast cancer cells

Stefano Fedeli DOTTORATO IN SCIENZE CHIMICHE - *Chimica*

P – 32. Assessment of a combined MM and QM approach for the study of the Single Molecule Magnet Fe₄ Ph adsorbed on Au(111)

Guglielmo Fernandez Garcia DOTTORATO IN SCIENZE
CHIMICHE - *Chimica*

P – 33. Spin-mixing interferometry with Bose-Einstein condensates

Marco Gabbrielli DOTTORATO IN FISICA E ASTRONOMIA -
Fisica

P – 34. Finite element method algorithm for the magma-rock interaction problem

Deepak Garg DOTTORATO IN SCIENZE DELLA TERRA

P – 35. Confocal light-sheet microscope for *in vivo* investigation of zebrafish neuronal and vascular systems

Ali Gheisari INTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS

P – 36. Electrodeposition, characterization and modeling of aluminium coatings

Andrea Giaccherini DOTTORATO IN SCIENZE CHIMICHE -
Chimica

P – 37. Characterization of metal sulphides thin films for photovoltaic application, obtained by means of electrodeposition and solvothermal synthesis.

Andrea Giaccherini DOTTORATO IN SCIENZE CHIMICHE -
Chimica

P – 38. Laboratory tests about resistivity variation in soil, in connection with root rate and soil humidity and bulk density

Yamuna Giambastiani DOTTORATO IN GESTIONE SOSTENIBILE DELLE RISORSE AGRARIE, FORESTALI E ALIMENTARI -
Ingegneria Agro-Forestale (IAF)

P – 39. Size distribution and Rare Earth Elements determination in arctic aerosol

Fabio Giardi DOTTORATO IN SCIENZE CHIMICHE - *Chimica*

P – 40. Photosynthesizing on metal excess: copper differently induced changes in various photosynthetic parameters in copper tolerant and sensitive *Silene paradoxa L.* populations

Elisabetta Giorni DOTTORATO IN BIOLOGIA - *Biologia Vegetale*

P – 41. Multimodal nonlinear microscopy applied to the study of tissue lesions

Cristina Giubani INTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS

P – 42. Self-assembly, stability and performances of water-based cleaning systems

Martina Guidotti DOTTORATO IN SCIENZE CHIMICHE -
Chimica

P – 43. A study on well integrity in a natural analogue for the geological CO₂ storage

Ana Hernandez-Rodriguez DOTTORATO IN SCIENZE DELLA
TERRA

P – 44. Isoxazol-5-(2H)-one derivatives as human neutrophil elastase (HNE) inhibitors

Antonella Iacovone DOTTORATO INTERNAZIONALE IN AREA
DEL FARMACO E TRATTAMENTI INNOVATIVI - *Scienze
Farmaceutiche*

P – 45. Semi-synthetic strategy to obtain aberrantly N-glycosylated Myelin Oligodendrocyte Glycoprotein as a specific autoantigen of multiple sclerosis

Matthaia Ieronymaki DOCTORATE IN CHEMICAL SCIENCES
(UNIVERSITY OF CERGY-PONTOISE)

P – 46. Bindi's grapevine model implementation: phenology, biomass partitioning and nitrogen balance

Luisa Leolini DOTTORATO IN SCIENZE AGRARIE E
AMBIENTALI

P – 47. Non-SELEX: a valuable tool for aptamer selection. The case of tau protein.

Samuele Lisi DOTTORATO IN SCIENZE CHIMICHE - *Chimica*

P – 48. Effect of different agricultural management on ants community in organic and non organic vineyards

Alberto Masoni DOTTORATO IN BIOLOGIA - *Etologia ed Ecologia*

P – 49. The redox-dependent folding state of human Cox17 visualized by in-cell NMR

Eleonora Mercatelli INTERNATIONAL DOCTORATE IN STRUCTURAL BIOLOGY

P – 50. Predictive modelling for dairy cow welfare assessment

Riccardo Moretti DOTTORATO IN SCIENZE AGRARIE E AMBIENTALI

P – 51. Antimicrobial activity of Auranofin

Carlotta Morichi DOTTORATO IN BIOLOGIA - *Genetica e Microbiologia*

P – 52. Improving thermal performance of earth-to-air heat exchanger by wetting the ground: an experience in Southern Iraq

Wasseem Morshed DOTTORATO IN GESTIONE SOSTENIBILE
DELLE RISORSE AGRARIE, FORESTALI E ALIMENTARI -
Ingegneria Agro-Forestale (IAF)

P – 53. The click chemistry approach for the
development of selective carbonic anhydrase inhibitors

Alessio Nocentini DOTTORATO INTERNAZIONALE IN AREA DEL
FARMACO E TRATTAMENTI INNOVATIVI - *Scienze Farmaceutiche*

P – 54. Multivariate approach for screening and
optimization of RP-UPLC method performance for a
formulated vaccine.

Luca Nompri DOTTORATO INTERNAZIONALE IN AREA DEL
FARMACO E TRATTAMENTI INNOVATIVI - *Scienze Farmaceutiche*

P – 55. Self-folding microstructures with active liquid
crystalline part

Dmitry Nuzhdin INTERNATIONAL DOCTORATE IN ATOMIC
AND MOLECULAR PHOTONICS

P – 56. Generating solitons on discrete Heisenberg
chains and how to manipulate qubits with them

Davide Nuzzi DOTTORATO IN FISICA E ASTRONOMIA - *Fisica*

P – 57. Cancer stem cells in osteosarcoma

Gaia Palmi DOTTORATO IN SCIENZE CLINICHE - *Patologia e
Clinica dell'Apparato Locomotore e dei Tessuti Calcificati*

P – 58. A theory of River Restoration through mitigation of hydrogeological risk

Alexander Palummo DOTTORATO IN ARCHITETTURA -
Progettazione Urbanistica e Territoriale

P – 59. Development of innovative systems for cleaning and protection of Cu-based metallic artifacts

Erica Isabella Parisi DOTTORATO IN SCIENZE CHIMICHE -
Scienza della Conservazione dei Beni Culturali

P – 60. Mimicking serin protease inhibitor H1 chaperone function in collagen biosynthetic pathway via the template assembled synthetic protein approach

Simona Pascarella DOTTORATO INTERNAZIONALE IN AREA DEL FARMACO E TRATTAMENTI INNOVATIVI - *Farmacologia, Tossicologia e Trattamenti Innovativi*

P – 61. Vibrational landscape on the nest of *Polistes dominula*

Irene Pepiciello DOTTORATO IN BIOLOGIA - *Etologia ed Ecologia*

P – 62. The diagnostic boundary between autism spectrum disorder, intellectual developmental disorder and schizophrenia spectrum disorders

Micaela Piva Merli DOTTORATO TOSCANO DI NEUROSCIENZE

P – 63. Genome-scale metabolic reconstruction of *Acinetobacter baumannii* species

Luana Presta DOTTORATO IN BIOLOGIA - *Genetica e Microbiologia*

P – 64. Partition functions and stability criteria of topological insulators with non-Abelian edge excitations

Enrico Randellini DOTTORATO IN FISICA E ASTRONOMIA - *Fisica*

P – 65. DNA technology for small molecules sensing: a new approach for acetamiprid detection

Riccardo Rapini DOTTORATO IN SCIENZE CHIMICHE - *Chimica*

P – 66. Core-shell nanoparticles for DNA delivery actuated by magnetic fields

Annalisa Salvatore DOTTORATO IN SCIENZE CHIMICHE - *Chimica*

P – 67. Early environmental therapy rescues brain development in a mouse model of Down Syndrome

Gabriele Sansevero DOTTORATO TOSCANO DI NEUROSCIENZE

P – 68. Anion complexes with tetraazine-based ligands

Matteo Savastano DOTTORATO IN SCIENZE CHIMICHE -
Chimica

P – 69. High-pressure chemistry in nanoconfined systems: polyCO and 1D-PolyAcetylene/Zeolites nanocomposites

Demetrio Scelta INTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS

P – 70. A generalized sense of number

Irene Togoli DOTTORATO TOSCANO DI NEUROSCIENZE

P – 71. Investigation of the structural properties of MgO-based eco-sustainable cements and assessment of innovative strategies for their improvement

Monica Tonelli DOTTORATO IN SCIENZE CHIMICHE - *Chimica*

P – 72. Highly dispersed Ni catalysts over Cerium modified mesoporous MCM-41 for hydrogen production by ethanol steam reforming

Jorge Tovar Rodriguez DOTTORATO IN SCIENZE CHIMICHE -
Chimica

P – 73. Fisher vectors over random density forests for object recognition

Francesco Turchini DOTTORATO IN INGEGNERIA
DELL'INFORMAZIONE - *Informatica*

P – 74. Climate, cities and bioenergy: development of indicators for sustainable management

Leonardo Verdi DOTTORATO IN SCIENZE AGRARIE E
AMBIENTALI

P – 75. Nuclear magnetic resonance-based metabolomics approach to study urines of chronic inflammatory rheumatic diseases patients

Alessia Vignoli INTERNATIONAL DOCTORATE IN STRUCTURAL
BIOLOGY

P – 76. Chelating agents and sensors for transition metal cations

Rania Zartit DOTTORATO IN SCIENZE CHIMICHE - *Chimica*

Poster abstracts

Poster

Ciclo XXIX

Integrating field survey on geo-environmental factors
and orthophoto information to monitor coastal dune
habitats – A pilot study to evaluate coastal dune
vulnerability

Fernanda Alquini

DOTTORATO IN SCIENZE DELLA TERRA - Dipartimento di Scienze della Terra (DST)

ENVIRONMENT, RESOURCES AND SECURITY, NATURAL HAZARDS

Vegetation works like an obstacle, deforms air flow and prevents sediment transport causing the decrease of the energy transfer. The aim of this study is to integrate abiotic and biotic data to develop a vulnerability index of coastal dunes. The research has been planned in two pilot sites: Migliarino San Rossore Regional Park in Italy and Acarai National Park in Brazil. In both sites, the following data will be collected: coverage of the different plant communities; geomorphological and sedimentological information; acquisition of a set of environmental parameters by means of wireless sensor technology. Preliminary results are coming from the Italian site. The San Rossore Park has been split in two areas basing to their different characteristic. The southernmost area, which is subject to strong erosional processes, is characterized by the predominance of forest vegetation (71 %), followed by fixed dunes (13.16 %), hygrophilous vegetation (0.78 %), water areas (0.01 %), and bare soil (1.95 %). The pioneer yearly vegetation is absent due to the coastal erosional processes. On the other hand, the northernmost site is dominated by vegetation of fixed dunes (41 %), followed by *Juniperus* assemblages (24.15 %), annual communities of upper beach (8.92 %), hygrophilous vegetation (3.35 %), bare soil (2.31 %), pathway (2.19 %), and water areas (1.32 %).

Poster

Ciclo XXX

Climosequence approach to monitor the effects of
exposure and altitude on physical, chemical and
microbial properties of alpine soils

Tommaso Bardelli

DOTTORATO IN SCIENZE AGRARIE E AMBIENTALI - Dipartimento di Scienze
Produzioni Agroalimentari e dell'Ambiente (DISPAA)

FORESTRY, CELLULAR BIOLOGY

To monitor the microclimate effects on soil microbial properties, it is of paramount importance to link two of the principal indicators of soil quality and functionality, i.e. microbial biomass and enzymatic activities. This study focuses on a climosequence approach to evaluate the impact of altitude and exposure on soil properties in ten alpine sites in Trentino (Italy). A total of 450 samples were collected in August 2012. Three plots located at 50 m from each other were set-up in each site and five sub-samples were randomly collected at three soil depths. We performed a multiple-enzymatic assay to detect eight hydrolases that are representative of the principal biogeochemical cycles. Microbial biomass was comparatively assessed by using two different DNA extraction methods: extraction-purification of soil DNA with a commercial kit to obtain a pure DNA for fingerprinting analysis; direct extraction-quantification of crude soil DNA. The second method provided a reliable estimator of microbial biomass. Microbial biomass and enzymatic activities decreased significantly with soil depth, whereas altitude and exposure effects were often masked by the site effect. Moreover, our results suggested a significant and positive correlation between microbial biomass and all enzyme activities studied in the Alpine soils.

Poster

Ciclo XXX

Development of a nonlinear multimodal microscopic platform and its application to the study of arterial tissues

Enrico Baria

INTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS -
Laboratorio Europeo di Spettroscopie non Lineari (LENS)
MICROSCOPY, OPTICS AND PHOTONICS, BIOPHYSICS

I developed a nonlinear multimodal laser-scanning microscope for acquiring Second Harmonic Generation (SHG), Two-photon Excitation Fluorescence (TPEF) and Fluorescence Lifetime Imaging Microscopy (FLIM) images. Such a microscope was used in order to study *ex vivo* arterial tissue samples affected by atherosclerosis (that is, an accumulation of fatty material - cholesterol, triglycerides - within the arterial wall) without any staining or labeling. The acquired images were analyzed through three techniques: Fast Fourier Transform (FFT), Grey-level Co-occurrence Matrix (GLCM) and fluorescence lifetime. Using this approach, it was possible to discriminate arterial wall regions from lipid depositions on the basis of their anisotropy ratio, correlation length and fluorescence decay parameters. Therefore this study suggests a high-resolution, label-free and noninvasive alternative to standard histological and immunohistochemical analysis of arterial tissues affected by atherosclerosis.

Poster

Ciclo XXIX

Nano- and microcapsules: synthesis and physical chemical characterization.

Arianna Bartolini

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

PHYSICAL CHEMISTRY-CHEMICAL PHYSICS, DRUGS-HEALTH, POLYMER SCIENCE

The aim of this PhD project concerns the synthesis and the physical chemical characterization of polymeric nano- and microcapsules. This is of paramount applicative relevance considering the growing search for confinement and delivery systems in several areas. Micro-encapsulation is a powerful technique to shield an active product from the surrounding environment. A suitable shell encloses the functional ingredient; the barrier can either confine the active material and that can regulate its release behavior by controlling its diffusion through the wall or by triggering responsive shells. Furthermore the confinement of certain types of substances can be useful either to prevent undesired interactions, or to deliver the active, or to delay their reactions until needed. As a result, the uses of micro-encapsulation are countless, ranging from cosmetics, detergents, targeted drug delivery systems to food additives. Different types of capsules are synthesized, by using different polymers and different formulations, with the final goal to encapsulate a wide range of substances. Several parameters have been tuned to optimize the capsules preparation procedure. Capsules are investigated by Dynamic Light Scattering (DLS), Small Angle X-ray Scattering (SAXS) and by confocal and optical microscopy.

Poster

Ciclo XXVIII

New acridine based ligands for metal ion binding and fluorescence sensing

Francesco Bartoli

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

INORGANIC CHEMISTRY, ANALYTICAL CHEMISTRY, SPECTROSCOPY

There is a growing interest for new fluorescent ligands capable to bind selected metal ions, due to their potential use for metal cation sensing in biological or environmental matrices. In this context, we have synthesized two new chelating agents containing an acridine fluorophore and two 1,4,7-triazonane (L1) or 1,4,7-trithia-10-azacyclododecane (L2) units as binding site for metals. Metal binding was analyzed by coupling potentiometric titrations and UV-vis and fluorimetric measurements. Ligand L1 is able to selectively sense in aqueous media Zn(II) over transition, post-transition, alkali and alkaline metal cations, thanks to a marked increase of the emission observed upon Zn(II) binding. The emission is not only determined by metal binding, but also by pH, the Zn(II) complex being strongly emissive at neutral or slightly acidic pH values. L2 is able to sense Cd(II) and presents a different pH dependence of the emission of the complexes. These results will be discussed considering the different binding ability of the chelating sites of L1 and L2 not only for metal cations but also for acidic protons.

Poster

Ciclo XXIX

Microwave assisted pyrolysis of biomass

Mattia Bartoli

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

ANALYTICAL CHEMISTRY, FORESTRY

In the last century consumption of fossil resources imposed to find alternative renewable sources to satisfy the requests for energy and chemical. For this reason biomasses were become the most interest field to research new way to produce fuels and chemicals with low environmental impact from renewable feedstocks. Ligno-cellulosic biomasses are the most available natural and renewable resources, and its composition and attractive properties make it a very valuable product. A very promising way to performed it is use of pyrolytic methodology. Pyrolysis methods are very promising to avoid pollution due to combustion of biomass residual. A great number of pyrolytic treatments of biomass were development in the years using different reactors and conditions. Recently biomass microwave assisted pyrolysis (MAP) gained a particular interest because of the speed of the process and the quality of the products obtained despite the drawback of employ a microwave (MW) absorbent. Biomass can be absorb and MAP of biomass can be performed without MW absorber but an absorber can be used to improve the quality of products and to reduce process time. In this framework is shown the results of different MAP of biomass and methods employed to define the characteristics of products obtained.

Poster

Ciclo XXVIII

Novel non-aqueous amine solvents for reversible CO₂ capture

Francesco Barzagli

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

INORGANIC CHEMISTRY, ENVIRONMENTAL / POLLUTION

Aqueous alkanolamines have a long story as efficient systems for CO₂ separation in ammonia and hydrogen plants, biogas upgrading, natural gas sweetening and gas refinery. Recently, these aqueous sorbents have been also studied for application on CO₂ removing from industrial exhaust streams. However, the high operating costs associated mainly to the thermal regeneration of the sorbents (because of the stability of both bicarbonate and amine carbamate and heat capacity of water), to the amine decomposition and evaporation, as well as to the equipment corrosion, are the major obstacles to extensive application in large scale commercial plants. In an effort to preserve the high efficiency of aqueous alkanolamines while reducing their disadvantages, we have devised the strategy to replace water with organic solvents or to avoid any solvents, in order to redirect the reaction of CO₂ capture towards less stable carbonated species which thereby require lower regeneration temperature at room pressure. We have formulated different sorbents that may have some crucial advantages: lower amine decomposition, reduction of the equipment corrosion and a considerable decrease of the regeneration heat penalty. Additional advantages of solvent-free amines are the reduced amount of the absorbent and no energy is wasted to heat solvent.

Poster

Ciclo XXX

Electrodeposition from Ionic Liquids (IL) and Deep Eutectic Solvents (DES)

Enrico Berretti

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

SURFACE SCIENCE, ELECTROCHEMISTRY

The ever rising concerns about the environmental impact of water based industrial electrodeposition processes are pushing the quest for alternative electrolytes. Recently Ionic Liquids and Deep Eutectic Solvents have been considered, leading to a variety of electroplating solutions for obtaining coatings of a wide variety of metals and alloys. Nevertheless the full technological exploitation is still limited. Just a few commercial electrodeposition processes not employing water electrolyte are actually known. This is mostly because of the physical and chemical properties of such electrolyte that have complex implication in both the quality of the coating and the management of the electroplating solutions. To overcome the present limitations the research in the field of non-aqueous electrodeposition still has a number of open issues both on the side of fundamental science and technological aspects. My study focuses on the development of novel electrochemical methods for the deposition of metal coatings in Ionic Liquids and Deep Eutectic Solvents to give a contribution to the understanding of the basics of the electrochemical growth in such electrolytes, with a special emphasis for the production of coatings using metals whose electrodeposition cannot be achieved in water medium.

Poster

Ciclo XXIX

Italian adaptation of the Parental Attitudes Scales**Giuly Bertoli**

DOTTORATO IN SCIENZE CLINICHE - Psicologia e Terapia del Dolore - Dipartimento di Scienze della Salute (DSS)

PSYCHOLOGY

Introduction: the present study explored the psychometric properties of the Italian version of the Parental Attitude Scales (PAD). The PAD are a 46-item self-report questionnaire that was developed to assess three parental attitudes dimensions: Pleasure-Displeasure, Arousal-Non Arousal, Dominance-Submissiveness. Methods: 483 parents (235 males; mean age = (42.9 ± 6.1) years) completed the PAD and measures of theoretically and conceptually related constructs. A sub-sample of 59 participants completed the PAD twice in order to explore the test-retest reliability. Results: the results from Principal Axis Factoring (PAF) did not support the original three-factor solution. Indeed, the three factors explained the 22.9% of the total variance; the factor loadings were low, and considering the correlation matrix, many items have saturated on each factor. Internal consistency was moderately acceptable, temporal stability and concurrent validity was questionable. Conclusions: the Italian version of the PAD showed a lot of weaknesses from a psychometric point of view. Further studies are needed to explore and evaluate a short version of the Parental Attitudes Scales in the Italian sample.

Poster

Ciclo XXIX

6-aminopyridine-3,5-dicarbonitriles as non-nucleoside adenosine A1 receptor agonist

Marco Betti

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- Scienze Farmaceutiche - Dipartimento di Neuroscienze, Psicologia, Area del Farmaco
e Salute del Bambino (NEUROFARBA)

ORGANIC CHEMISTRY, DRUGS-HEALTH, PHARMACOLOGY, NEUROSCIENCE

The adenosine A1 receptor is the most extensively investigated of the adenosine receptor (AR) family that also includes the A2A, A2B and A3 subtypes. Many different classes of ligands were evaluated at the A1AR and to date several recurring structural features have been identified for defining the affinity or efficacy of the target compound. For a long time, the A1 agonist profile has been associated to compounds with an adenosine-like structure. In contrast, recent studies reported some non-nucleoside compounds belonging to the 6-aminopyridine-3,5-dicarbonitrile series that show different degree of efficacies at the different ARs. Some of these, thought lacking the ribose moiety, have significant affinity and efficacy at the A1AR. A1AR agonists exerted anti-nociceptive effects at the spinal cord level thus leading to hypothesize their potential for the treatment of neuropathic pain. On this basis, a series of 6-amino-4-heteroarylpyridine-3,5-dicarbonitriles were designed as A1 agonists which were evaluated for their affinity and efficacy at the A1AR subtype. Most of the synthesized compounds are endowed with A1 binding affinity in the nanomolar range, high selectivity and an agonist profile. Selected compounds are being tested in an *in vitro* model of neuropathic pain in order to evaluate their anti-nociceptive potential.

Poster

Ciclo XXX

Multi-level Modeling of Lanthanide-containing materials by *ab initio* methods

Matteo Briganti

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

INORGANIC CHEMISTRY, MATERIAL SCIENCE, PHYSICAL CHEMISTRY-CHEMICAL PHYSICS, COMPUTATIONAL MODELING

An *ab initio* characterization of single molecule magnets containing lanthanide atoms by a multiconfigurational post-Hartree-Fock method is proposed. A detailed description of the magnetical and optical properties implies a reliable computation of the excited states of the molecule. Therefore relativistic effects, as spin-orbit coupling, and electronic correlation have to be considered. For these reasons, a method in which a relativistic hamiltonian combined with the multi-configurational approach is mandatory in order to treat electronic correlation and spinorbit coupling, respectively. However, fine geometrical effects are responsible of magnetic properties in such compounds and a deep analysis on this topic is still missing, therefore compounds have been studied in order to verify if this computational protocol could also be able to account for finest effects such as the rotations of the main magnetic axis due to the rotation of the atoms in the first coordination sphere. Indeed we want to set a computational protocol suitable for isolated or periodic systems containing lathanides ions and shed light on the ligand field effect on them in order to extrapolate useful and generally applicable magneto-structural correlations to understand how electronic structure can influence magnetic behaviour, optical properties and relaxation mechanisms.

Poster

Ciclo XXX

QCL-based metrological-grade THz spectroscopy tools

Annamaria CampaINTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS -
Dipartimento di Fisica e Astronomia

MATERIAL SCIENCE, OPTICS AND PHOTONICS, METROLOGY

The Terahertz region of the electromagnetic spectrum covers a still under-explored gap, though having potential not only for countless applications in strategic fields, like bio-medical diagnostics, communication technology, security and defense, but also for a number of studies on molecules, since rotational transitions generally fall in the far-infrared range. These transitions typically have large line-strengths, and can be very suitable not only for the development of high-sensitivity trace-gas sensing techniques, but also for investigating fundamental aspects in molecular physics. High precision THz molecular spectroscopy therefore promises amazing scientific and technological applications, provided that sources with suitable high power, wide tunability and narrow linewidth, such THz Quantum Cascade Lasers are available. The first application of a QCL phase-locked to a free-standing THz Frequency Comb Synthesizer (FCS) was recently demonstrated, achieving a state-of-the-art accuracy of 4×10^{-9} in the determination of the absolute frequency of a THz transition. Saturated-absorption spectroscopy, and the possibility to use well-established spectroscopic tools, such as cavity resonators, are the natural evolution of experimental setups aiming to overcome the limitation set by the Doppler broadening of molecular lines at room temperature, paving the way to next generation THz metrological tools.

Poster

Ciclo XXX

Evaluation of diaphragm thickening by diaphragm
ultrasonography: a reproducibility and repeatability
study

Iacopo Cappellini

DOTTORATO IN SCIENZE CLINICHE - Scienze Anestesiologiche e Chirurgiche -
Dipartimento di Medicina Sperimentale e Clinica

BIOINFORMATICS, ULTRASONOGRAPHY

Background: ultrasonography is a fascinating tool for diaphragm functional analysis. Bi-dimensional mode (B-mode) and time-motion (M-mode) are two useful way to study the zone of apposition (ZOA) of the diaphragm, between the lung and liver on the right side and the lung and spleen on the left one. Methods: 10 healthy volunteers were enrolled and studied by three operators with different skills in ultrasonography. Left and right hemi-diaphragms of every individual have been scanned randomly by each operator three times both in B-mode and in M-mode. In a second step, a fourth operator has calculated the thickening fraction (TF), by the formula $TF = (TEI - TEE)/TEE$. TEI is thickness at end inspiration and TEE thickness at end expiration. Then, we conducted a gage R&R ANOVA analysis on TF, to determine %R&R index, with an acceptable threshold less than 30%. Results: B-mode has resulted more accurate than M-mode in determining TF, regardless of side assessed (%R&R 0.24 vs 0.33 respectively). Moreover, B-mode assessment on the right hemidiaphragm was associated with a minor degree of variability (%R&R 0.27). Conclusions: ultrasound scan of the ZOA is closely related to skills of operators involved; therefore it is crucial that scans should be performed by clinicians with similar competences in ultrasonography.

Poster

Ciclo XXX

Fast analysis of glibenclamide and its related substances by capillary electrophoresis

Claudia Caprini

DOTTORATO INTERNAZIONALE IN AREA DEL FARMACO E TRATTAMENTI INNOVATIVI
- Scienze Farmaceutiche - Dipartimento di Chimica "Ugo Schiff"

ANALYTICAL CHEMISTRY

A fast and reliable capillary zone electrophoresis method was set up for the simultaneous determination of glibenclamide (GLI), an antidiabetic drug belonging to the class of sulfonylureas, and its main impurities reported in European Pharmacopeia. The method was developed following QbD principles according to ICH guideline Q8, implementing each step of QbD workflow for separation methods as recently reported. The analytical target profile was defined by the baseline separation and the accurate determination of GLI and its impurities in the pharmaceutical dosage form, with LOQ values for the impurities equal or lower to 0.1% with respect to the main compound. In the screening phase different critical process parameters, each studied at three levels by a symmetric screening matrix, were taken into consideration: voltage, temperature, background electrolyte concentration and pH, injection time. The subsequent response surface study was carried out by using a Box-Behnken design and allowed the design space to be identified. By applying the selected working conditions, a complete separation of the analytes was obtained in less than 2 min. The developed method was validated according to ICH guideline Q2(R1) and then applied to the analysis of real samples of glibenclamide tablets.

Poster

Ciclo XXX

Trough territorial complexity: megacity and water uses**Benedetta Caprotti**DOTTORATO IN ARCHITETTURA - Progettazione Urbanistica e Territoriale -
Dipartimento di Architettura (DiDA)CULTURAL HERITAGE PRESERVATION, ENVIRONMENTAL / POLLUTION, ECOLOGY /
ETHOLOGY / EVOLUTION, ENVIRONMENT, RESOURCES AND SECURITY, URBAN
DESIGN, AGRICULTURE, FORESTRY

Water is priority resource in megacity's lifetime connected with million people subsistence. Look at geographical scale of megacity, the system for supply and wastewater isn't the only one involved. According to the theory of complexity based on relationship and interaction of anthropic and natural factors, start from ecological landscape approach the issue is to open a discussion above the circles of poverty connecting to water. How the relationship between the city and the cycle of water influence the landscape and the city socio-ecological structure? The objective of the research is to use water to look at the megacity; investigated the complexity at different layers and level. Undusted if the morphology linked to social character of water, how is explained throw traditional rules, social values and space, myth, can be useful to study and reduce megacity ecological problems. Case study 1. Mexico City founded in the middle of lake systems; it is now like a desert of two floor houses which sustainability is in danger. Has the Mexican megalopolis really compromised the older relationship between his territory and the neighbours region? Can the local water traditions and technique be re-involve in the management of water in a sustainably ethics prospective?

Poster

Ciclo XXVIII

2D-Fluorescence studies of neat binding media and simulated paint mixtures

Serena CarlesiDOTTORATO IN SCIENZE CHIMICHE - Scienza della Conservazione dei Beni Culturali -
Dipartimento di Chimica "Ugo Schiff"

ANALYTICAL CHEMISTRY, CULTURAL HERITAGE PRESERVATION, SPECTROSCOPY

Spectrofluorimetric analysis of binding media can be particularly useful, because organic materials employed in paintings are often fluorescent and binding media from different sources have different fluorescence spectral profiles. In this work, fluorescence excitation-emission maps were acquired for the analysis of traditional binding media used in paintings such as drying oils (linseed oil, walnut oil, poppy oil and stand-oil derived from linseed oil), proteinaceous materials (egg yolk, egg white, whole egg, casein, rabbit skin glue, strong glue and fish glue) and polysaccharides (arabic gum and tragacanth gum). Furthermore, the presence of a pigment was investigated. Since pigments co-exist with and may be linked to binding media in paintings, analysis is often complicated due to pigment-binder interactions which can be both chemical and physical. So, paint samples based on lead white (basic lead carbonate) were prepared with different binders, egg-based, casein, linseed oil and poppy-seed oil. Each sample was individually applied as a thick film on a microscope glass slide and left to dry at least one year before analysis. 2D-Fluorescence provides distinct advantages for understanding the complex mixture of fluorophores in binding media. Moreover the excitation-emission maps often convey information on the extent of sample aging and degradation.

Poster

Ciclo XXX

Matarka: a new ungrouped iron meteorite from Morocco

Vanni Moggi Cecchi

DOTTORATO IN SCIENZE DELLA TERRA - Dipartimento di Scienze della Terra (DST)

MICROSCOPY, MINERALOGY AND PETROLOGY

At least 43 small sized fragments of a newly discovered iron meteorite have been recovered near the locality of Matarka, in the Moroccan desert in 2014. The study of the location of the coordinates of the recovered fragments suggests the presence of a strewn field. One of these fragments was brought to Italy by Mario di Martino of OATO-INAF and analyzed at the Dipartimento di Scienze della Terra and Dipartimento di Chimica by means of optical microscopy and SEM to check textural and compositional features. Taenite displays a markedly high nickel content, ranging from 14 to 25 Wt % Ni. A distinct Widmanstaetten pattern has been detected, with a kamacite lamellae width ranging from 0.2 to 0.3 mm. ICP-MS analyses performed at the Department of Earth and Atmospheric Sciences of the University of Alberta, Canada, provided interesting results. The very high Ni, Ga, Ru, Pd and Pt, but relatively low Ir contents, indicate that the meteorite does not fit into any presently known groups, suggesting a possible classification as ungrouped iron meteorite. The meteorite has been sent to the Meteoritical Society for approval.

Poster

Ciclo XXX

Glycosylated natural saponins for autoantibody recognition

Anne-Sophie Champy

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

DRUGS-HEALTH, NMR, SAPONINS, AUTOIMMUNE DISEASE

In the field of the search for plants with saponins according to chemotaxonomic criteria (e.g. family and genus already known for their high heterosidic secondary metabolites), several known plants could be again discovered such as alimentary (*Allium*) and ornamental plants or traditional desertic plants with sulfated glycosides. Saponins, with their heterosidic and amphiphilic structure, are able to settle on cell membrane in order to form pore. The chemical study of saponins involve the use of large extraction and chromatographic techniques. Their spectral analysis is complex, based mainly on bidimensional NMR (nuclear magnetic resonance) at 600 MHz and mass spectrometry. Plants, rich in saponins, are used in Phytotherapy but rarely pure saponins in spite of their various pharmacologic activities *in vitro*, due to their potential toxicity. The use of saponins as diagnostic tool is an original alternative. An N-glycosylated peptide has demonstrated yet a good efficiency in recognition of specific autoantibodies in patient's sera with multiple sclerosis and with Rett syndrome. The aim of this project is to use natural saponins or conjugated saponins with peptides to detect serum biomarkers in different neurodegenerative autoimmune disease.

Poster

Ciclo XXIX

Exploring the genetic basis of symbiotic performance
in rhizobia: the *acdS* gene in *Sinorhizobium meliloti*

Alice Checcucci

DOTTORATO IN BIOLOGIA - Genetica e Microbiologia - Dipartimento di Biologia
(BIO)

BIOINFORMATICS, CELLULAR BIOLOGY, RECOMBINANT PROTEINS, MOLECULAR
BIOLOGY

Mutualistic cooperation is one of the most fascinating issue in evolutionary biology and legume-rhizobia symbiosis represent models of cross-kingdom mutualism. However, not all strains of the same rhizobial species have the same mutualistic phenotype, and only few studies explore the genetic basis of these differences. In this context, one of the most intriguing gene is that encoding the enzyme 1-aminocyclopropane-1-carboxylate (ACC) deaminase (*acdS*), present in the dispensable genome of *Sinorhizobium meliloti* species, that could be involved in the sequestering and cleaving of the plant-produced stress hormone ethylene. Since the role of *acdS* in the mutualistic and symbiotic behavior is not completely clarified, a phylogenetic and comparative genomic analysis of *acdS* orthologs has been performed in genomes of *S. meliloti* strains and functional studies have been carried out by expressing *acdS* in the model strain *S. meliloti* Rm1021, which lacks *acdS* gene. Then, the symbiotic and endophytic phenotypes of recombinant vs parental strain have been evaluated in terms of competition for root nodule occupancy, plant colonization and modulation of ethylene production by the host plant. Data showed that *acdS* orthologs in *S. meliloti* are polyphyletic and may indeed derive from different alphaproteobacteria. No increase in fitness for nodule occupancy was found, but a modulation of ethylene levels was detected in plant infected by *acdS*-expressing strain. We conclude that *acdS* in *S. meliloti* could be more related to the endophytic life-style than to the symbiotic interaction.

Poster

Ciclo XXVIII

Synthesis and characterization of new materials for technological and solar devices

Serena Cinotti

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

MATERIAL SCIENCE, SURFACE SCIENCE

Semiconductors with application in the photovoltaic field were prepared by electrodeposition. In particular, we used the E-ALD (Electrochemical Atomic Layer Deposition) method to build a p-n junction. Furthermore, SXRD (Surface X-Ray Diffraction) investigations were undertaken with the aim of performing a structural characterization of the grown films. E-ALD is a layer-by-layer electrodeposition based on the alternate underpotential deposition (UPD) of atomic layers of the elements constituting a compound. The starting point was the deposition of the p semiconductors, (Cu-Zn-S), prepared alternating the UPD of the binary sulfides, CuS and ZnS. After the optimization of the deposition condition of the p films, the electrochemistry behavior of the Cd solution on the substrate covered by the p films has been studied, to perform the deposition of the n film (CdS). Once determined the UPD of Cd, same samples were analyzed by XPS (X-Ray Photoelectron Spectroscopy). Furthermore, in situ SXRD measurements performed at ESRF (Grenoble), allowed to investigate the growth mechanism of Cu-Zn-S thin films. The growth of the film was monitored by following the evolution of the Bragg peak. Analysis of these data are still in progress but the samples show crystallinity, proposing E-ALD as method to grow structurally ordered thin films.

Poster

Ciclo XXX

The landscape as an orienting factor in *Talorchestia
martensii*

Alice Ciofini

DOTTORATO IN BIOLOGIA - Etologia ed Ecologia - Dipartimento di Biologia (BIO)

ENVIRONMENTAL / POLLUTION, ECOLOGY / ETHOLOGY / EVOLUTION

The equatorial sandhopper *Talorchestia martensii* uses several cues to return to the belt of damp sand of the beach following the shortest route (the sea-land axis). The main references used in the zonal recovery are the sun and the geomagnetic field, even if the use of the sun at equatorial latitudes is not always possible because of its hourly azimuthal variation and the zenithal culmination. The aim of this work is to investigate the role of the landscape as a local orienting factor in this species. I tested adult individuals in a confined environment (a transparent plexiglass bowl) with and without the vision of the landscape of their home beach (Malindi, landward direction = 295°) and of a different-orientated shore (Temple Point, landward direction = 12°). Releases were carried out with either natural or zeroed magnetic field. Results show that individuals tested at Temple Point, in the periods in which the use of the sun is more difficult, orientate in good agreement with the sea-land direction indicated by the landscape. Therefore, the landscape seems to have great importance in the directional choice when the sun compass is not available.

Poster

Ciclo XXX

Melanocytic nevi and drugs: results of an observational study

Roberta Colucci

DOTTORATO IN SCIENZE BIOMEDICHE - Oncologia Sperimentale e Clinica -
Dipartimento di Scienze Biomediche, Sperimentali e Cliniche

DRUGS-HEALTH, MEDICINE, ONCOLOGY

Recent clinical and experimental findings suggest that the protracted assumption of some drugs might be associated with the risk of melanoma. Namely, it has been reported by preclinical or clinical studies that the assumption of β blockers, acetylsalicylic acid, omeprazole and statins might be protective toward melanoma onset and progression, while on the contrary the use of oral contraceptives (OC) or hormonal replacement therapy (HRT) seems to increase the risk of melanoma development. At present, no evaluation has been performed yet regarding their role in melanocytic nevi development. Thus, we performed an observational transversal study on patients referring to an outpatient for melanoma prevention, aiming to evaluate possible associations between the assumption of β blockers, acetylsalicylic acid, omeprazole, statins, OC and HRT with patients' melanocytic nevi total count. The results of our study, according to multivariate analysis, pointed out that the unique drugs associated with the total nevi count were OC or HRT. In particular, the use of such drugs was associated with an higher number of melanocytic nevi. According to our results, we suggest the women taking OC or HRT undergo regular dermatological skin evaluations for melanoma prevention, mostly in case of additional concomitant known risk factors for melanoma.

Poster

Ciclo XXVIII

Optical and electrochemical characterization of acridine ligands for sensoristic applications

Luca Conti

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

INORGANIC CHEMISTRY, ENVIRONMENTAL / POLLUTION

Arsenic and selenium play an important role in several environmental and health issues; while arsenic is an important contaminant of water (especially inorganic arsenite), selenium instead is an element present in trace amounts in most environmental and biological systems, indispensable in humans at trace levels but extremely toxic when taken in excessive doses. It is therefore evident how important would be to develop a simple and effective methodology for the environmental monitoring of both of these species. Our main goal, is to develop a selective and sensitive electrochemical sensor modified with some new acridine ligands for the determination of selenium and arsenic anionic species. For this purpose we have studied the ligand-anion interaction, through potentiometric and $^1\text{H-NMR}$ measurements, and investigated the electrochemical behavior of these anions through anodic and cathodic stripping voltammetry. In particular, we carried out the determination of Se(IV) both through redissolution technique of cathodic differential pulse voltammetry and via anodic voltammetry redissolution. Due to the specific chelating ability of these ligands, such techniques would be extremely promising in terms of selectivity and sensitivity in the determination of Se(IV) .

Poster

Ciclo XXIX

Generation of hybrid entanglement of light

Luca Costanzo

INTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS -
Laboratorio Europeo di Spettroscopia non Lineari (LENS)

OPTICS AND PHOTONICS

Entanglement between quantum and classical objects is of special interest in the context of fundamental studies of quantum mechanics and potential applications for quantum information processing. For example, the famous Schrödinger's cat is the main character of a paradox where entanglement with a microscopic quantum system (a radioactive atom) makes the poor macroscopic pet at the same time dead and alive. In quantum optics, a typical microscopic system is represented by a single photon while coherent states can be considered the most classical of pure states.

Recently, entanglement between a single photon and a coherent state in a free-traveling field was also identified as a useful resource for optical quantum information processing. However, the extreme difficulty involved in generating such states was highlighted, as it requires clean cross-Kerr nonlinearities. Here, we devise and experimentally demonstrate a scheme to generate such hybrid entanglement by implementing a superposition of two distinct quantum operations. The generated states clearly show entanglement between the two different types of states. Our work opens the way to the generation of hybrid entanglement of greater size and to the development of efficient quantum information processing using a new type of qubit.

Poster

Ciclo XXX

Involvement of central histaminergic system in the
oleoylethanolamide-induced antidepressant-like effect
in the mouse tail suspension test

Alessia Costa

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Psicologia, Area del Farmaco e Salute del Bambino (NEUROFARBA)

PHARMACOLOGY, TOXICOLOGY, NEUROSCIENCE

Major depression is the most common psychiatric disorder. Identifying new molecular targets for the pharmacotherapy of depression is crucial. Previous studies demonstrated that chronic administration of palmitoylethanolamide, an endogenous agonist of the peroxisome proliferator-activated receptor- α (PPAR- α), induced antidepressant-like effect in mice. We investigated PPAR- α as a possible target for the development of new antidepressant drugs by studying the effect of oleoylethanolamide (OEA), another endogenous PPAR- α agonist. Thus, we investigated if OEA possesses antidepressant-like effect using the tail suspension test (TST) a behavioural model predictive of antidepressant-like activity and whether this requires the integrity of the histaminergic system. Indeed, we previously observed that neuronal histamine (HA) participates to OEA-induced hypophagic effects. Normal (WT) and mice unable to synthesize histamine, were treated sub-chronically or chronically with OEA (5 or 10 mg kg⁻¹, i.p.) or vehicle (i.p.). OEA treatment induced dose-dependent reduction of immobility time when compared with vehicle-treated WT mice in both regimen. These effects were not observed in mice lacking neuronal histamine. These data suggest that the histaminergic system contributes to OEA-induced antidepressant-like effect in the TST and indicate that PPAR- α may be a target for the development of antidepressant drugs.

Poster

Ciclo XXIX

Aerobic oxidation of hydroxylamines to nitrones
catalyzed by a supported gold catalyst

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ORGANIC CHEMISTRY, MATERIAL SCIENCE

Traditional oxidants are often toxic and release considerable amounts of by products. As an alternative, oxygen is among the cheaper and less polluting stoichiometric oxidants, since it produces no waste or only water, thus following the principles of green chemistry. The implementation of a transition metal catalyst in combination with oxygen for the oxidation of alcohols to the corresponding carbonyl compounds represents an emerging more sustainable alternative to the traditional procedures. The related oxidation of disubstituted hydroxylamines to nitrones is much less studied. Nitrones are very useful building blocks for the synthesis of biologically active nitrogen containing compounds and can be obtained easily by oxidation of the corresponding hydroxylamines. Although bulk gold has for long time being regarded as poorly active metal, the surprisingly high activity of gold nanoparticle has prompted intensive research into their use for aerobic oxidation reactions. Dibenzylhydroxylamine was chosen as the model substrate in order to select the best conditions for the aerobic oxidation. We prepared the gold catalyst reducing tetrachloroauric acid with NaBH_4 in presence of silica, and the obtained Au silica catalyst was employed for the selective oxidation of other disubstituted hydroxylamines to the corresponding nitrones using different solvents only under air fluxing.

Poster

Ciclo XXIX

Raman measurements of hydrogen clathrate hydrate synthesized from liquid

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DOTTORATO IN FISICA E ASTRONOMIA - Fisica - Consiglio Nazionale delle Ricerche (CNR)

PHYSICAL CHEMISTRY-CHEMICAL PHYSICS, SPECTROSCOPY, MATTER PHYSICS

The nucleation and growth from the liquid phase of a solid clathrate-hydrate is a process even less understood and more difficult to study compared to that of a pure liquid. By means of *in situ* Raman spectroscopy, we have examined this phenomenon for the system hydrogen and water. Our sample is initially a liquid solution of hydrogen in water in contact with pressurized hydrogen gas at 2 kbar and at a temperature of 264 K (i.e. outside the stability region of common ice). After about 10 hours, we start to detect the vibrational spectrum of caged hydrogen molecules which increases in intensity while the solid clathrate grows. From the analysis of the Raman intensity, we can infer the population of the small (5^{12}) and large ($5^{12}6^4$) cages as a function of time during the hydrogen clathrate growth. Its behaviour, observed here for the first time, has some analogies with what observed in the more studied case of methane hydrate, where the small cages play a key role in the first stage of nucleation. However the possibility for hydrogen of multiple occupation of the large cages introduces an extra degree of freedom for the determination of the hydrate stoichiometry.

Poster

Ciclo XXVIII

Multi-target data association using sparse reconstruction

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COMPUTER VISION, MULTI-TARGET TRACKING, DATA ASSOCIATION

We describe a solution to multi-target data association problem based on l_1 -regularized sparse basis expansions. Assuming we have sufficient training samples per subject, our idea is to create a discriminative basis of observations that we can use to reconstruct and associate a new target. The use of l_1 -regularized basis expansions allows our approach to exploit multiple instances of the target when performing data association rather than relying on an average representation of target appearance. Preliminary experimental results on the PETS dataset are encouraging and demonstrate that our approach is an accurate and efficient approach to multi-target data association.

Poster

Ciclo XXX

Impairment of cell autophagy in primary CTSF/CLN13 cells

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Area del Farmaco e Salute del Bambino (NEUROFARBA)

NEUROSCIENCE, CELLULAR BIOLOGY

The neuronal ceroid lipofuscinoses (NCLs) are inherited neurodegenerative disorders characterized by accumulation of autofluorescent lipopigment in neurons and peripheral tissues. These genetically heterogeneous disorders share similar signs such as retinopathy with loss of vision, epilepsy and early cognitive decline. Onset is possible throughout life from infancy to adulthood (Kufs disease, KD). KD type B has recently been attributed to mutations in cathepsin F-CTSF/CLN13.

We characterized at the cellular level a novel mutation in CTSF associated with KD Type. The novel c.213+1G > C affects correct splicing, removing exon 1 and predicting a chopped N-terminus of CTSF, with a probable loss-of-function mechanism. N-terminus truncated forms of human CTSF has recently been associated with aggresome-like inclusions. Accordingly, we observed ultrastructurally aggresome-like structures in skin biopsies from three affected patients. These features were replicated in cultured fibroblasts where aggresome formation was confirmed in patients' fibroblasts using a specific detection dye. Western blotting analysis in cells lysate showed low amount of CTSF with higher levels of p62, LC3II and ubiquitin protein.

These results are suggestive of dysregulated autophagy and its involvement in triggering neuronal death in NCLs is considered to be prominent. Further investigations will clarify whether aggresome-like structures are present in CLN13 neuronal cells.

Poster

Ciclo XXX

Towards single-atom imaging in a strongly interacting Rydberg gas

Giulia Faraoni

DOTTORATO IN FISICA E ASTRONOMIA - Fisica - Dipartimento di Fisica e Astronomia

OPTICS AND PHOTONICS, ATOMIC PHYSICS

Rydberg atoms are atoms in high-lying energy states, characterized by a very large orbital radius (around $1\ \mu\text{m}$). It is responsible for their enormous dipole moments which result in strong long-range dipole-dipole interactions. Because of this property, cold atomic gases excited to Rydberg states can be used as quantum simulators of many-body systems with dipole-dipole interactions which are widespread in nature (condensed matter physics, chemistry, biology) but otherwise difficult to study because of the lack of control one has over them. When coherent light fields in appropriate configurations are coupled to a strongly interacting Rydberg gas, the peculiar properties of Rydberg atoms, such as the possibility of having only one Rydberg atom within a certain critical volume, give the chance to experimentally develop a non-destructive imaging technique, potentially able to spatially resolve a single Rydberg atom inside a random atomic gas. Among other applications, the presented imaging scheme could enable the study of dipolar energy transport phenomena, which play an important role in different fields, such as chemical reactions or photosynthetic light-harvesting complexes.

Poster

Ciclo XXVIII

Biotin-decorated carbon nanotubes as drug carrier to increase effect of doxorubicin against breast cancer cells

Stefano Fedeli

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ORGANIC CHEMISTRY, DRUGS-HEALTH, NANOMATERIALS

We have developed multiple-decorated carbon nanotubes (CNTs) as drug delivery system able to carry doxorubicin inside cancer cells. This result in an enhanced cytotoxic effect respect to the free drug. Decoration of the carbon nanotubes was accomplished through both covalent and non-covalent approaches: versatile click reactions and π - π interactions were exploited. To assess the internalization of the CNTs inside cells, a decoration with a fluorescent molecule, namely bodipy, was performed. Next, the nanotubes was decorated with a selector molecule, biotin, to increase the uptake of the system by cancer cells. The role of the selector was investigated by parallel biological test. Finally, the decorated system was loaded with the drug -doxorubicin-. Comparative studies were performed on the complete drug delivery system to highlight its effect respect to the free drug, as well as the contribute of the selector in the internalization efficiency.

Poster

Ciclo XXX

Assessment of a combined MM and QM approach for
the study of the Single Molecule Magnet Fe_4Ph
adsorbed on Au(111)

Guglielmo Fernandez Garcia

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INORGANIC CHEMISTRY, MATERIAL SCIENCE, SURFACE SCIENCE, PHYSICAL
CHEMISTRY-CHEMICAL PHYSICS, COMPUTATIONAL MODELING

An integrated MM (Molecular Mechanics) and DFT (Density Functional Theory) approach for the modelization of magnetic systems on surface has been developed and applied to the adsorption of single molecule magnet $[\text{Fe}_4(\text{L})_2(\text{dpm})_6]$ (Hdpm = dipivaloyl-methane and H_3L = 2-hydroxymethyl-2-phenylpropane-1,3-diol) or Fe_4Ph , on a surface of Au(111). These kind of systems are useful as model systems for the design of new materials, as spin valves or data storage devices. Indeed, the family of compounds of the Fe_4Ph exhibits a slow relation of the magnetization, making them suitable candidates for new technologies based on molecular magnetism. The DFT is the natural tool to study the electronic and magnetic properties, but becomes unaffordable if the interest lies also in the self-assembly process. We developed a full set of ad hoc classical potentials via the HESS2FF code and direct parametrization of specific interactions, to study large scale (temporally and spatially) phenomena. The new potentials have been tested on a series of benchmark to verify the reliability of the model. With this integrated approach we studied a single molecule on surface, the half coverage monolayer and the full coverage monolayer, identifying a new stable conformer and achieving important insights on the clusterization process.

Poster

Ciclo XXX

Spin-mixing interferometry with Bose-Einstein condensates

Marco Gabbrielli

DOTTORATO IN FISICA E ASTRONOMIA - Fisica - Dipartimento di Fisica e Astronomia

MATTER PHYSICS, ATOMIC PHYSICS

Measure is the key for our understanding of Nature: thanks to increasingly accurate measurements we have been able to investigate more outlying and fundamental phenomena. Historically and currently, one among the most powerful and precise techniques in metrology is interferometry. In a interferometer, two (light or matter) waves undergo a phase shift that generates observable interference effects: the aim of interferometry is measuring these effects in order to estimate the phase shift with the smallest possible uncertainty. Entanglement – the quintessence of quantum world – can be exploited to enhance the interferometric sensitivity and reach phase estimations with the highest accuracy permitted by Nature. Interferometry with trapped cooled atoms has come to the fore in the last decades because of its potential in ultraprecise measurement. In this direction, we explore the possibility to design a interferometer using Bose-Einstein condensates, which exploits entanglement generated by atom-atom interactions to perform phase estimation beyond the limitation of classical technologies, approaching the fundamental bound imposed by quantum theory.

Poster

Ciclo XXIX

Finite element method algorithm for the magma-rock interaction problem

Deepak Garg

DOTTORATO IN SCIENZE DELLA TERRA - Dipartimento di Scienze della Terra (DST)
COMPUTATIONAL MODELING, MATHEMATICS, FLUID DYNAMICS, SOLID, FLUID AND
MATERIALS MECHANICS, GEOCHEMISTRY AND VOLCANOLOGY

Magma dynamics in magma chamber causes new stress forces and deformations of rocks along the magma-rock interface. As a result rocks deform and elastic waves propagate, that are recorded at the earth surface as seismic signals. Interpretation of the recorded data is important for the quantitative assessment of volcanic processes and short-term risk evaluation. We are aiming to make a two way coupled finite-element method (FEM) for the simulation of dynamics of magma and the surrounding rocks. Magma is treated as a multicomponent and multiphase compressible fluid mixture. Its dynamics is characterised by Navier-Stokes equations for compressible flows in arbitrary Lagrangian Eulerian (ALE) frame of work. Rocks are treated as elastic isotropic materials. Their dynamics are characterised by the elastodynamics equation for solids in Lagrangian frame of work. The partial differential equations are numerically discretized by the space-time Galerkin FEM. The linear equations leaded by the FEM are solved by the LSQR solver. The simulation results of this method will help us to understand the link between the deep volcanic processes and the ground geophysical signals registered by the monitoring network.

Poster

Ciclo XXIX

Confocal light-sheet microscope for *in vivo*
investigation of zebrafish neuronal and vascular
systems

Ali Gheisari

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Laboratorio Europeo di Spettroscopie non Lineari (LENS)
MICROSCOPY, BIOPHYSICS

Leight-sheet microscopy has been introduced for biological study during last decade. Its characteristics such as large volume imaging, fast acquisition and photobleaching reduction made this technique as a unique microscope to investigate big biological tissues (e.g. mouse brain). We have set up a light-sheet microscope for *in vivo* imaging of zebrafish larva. Here the neuronal and vascular system of zebrafish larva has been studied. The result provide information about the heart beating, cerebrovascular structure, neuronal structure and neuronal activity.

Poster

Ciclo XXX

Electrodeposition, characterization and modeling of aluminium coatings

Andrea Giaccherini

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

MATERIAL SCIENCE, PHYSICAL CHEMISTRY-CHEMICAL PHYSICS, COMPUTATIONAL
MODELING

By means of electrodeposition in aqueous solutions it is not possible to obtain films of metal such as Aluminium, Tin, Tantalum and Magnesium, this is mainly due to the small electrochemical stability window of water. The aim of the project is to study metal coatings by means of electrodeposition from ionic liquids, in particular for Aluminium, likely has come the time for the developing of a full scale industrial process. The main objective of my work is to formalize a complete computational model of the electrodeposition process, in the sense of a dynamical model of the continuous domains and variables present in the electrochemical cell at a macroscopic level. A common approach to these kind of simulation is the Finite Elements Analysis (FEA), which is a strategy to solve the governing partial differential equation time and space dependent, by means of a suitable discretization. Physical parameters to model the transport and chemical kinetics phenomena, will be determined by means of electrochemical measurements and quantum mechanical calculations. After validation by means of a comparison with experimental data, the model will be useful for an *a priori* optimization of the anodes geometry in specific coatings applications.

Poster

Ciclo XXX

Characterization of metal sulphides thin films for photovoltaic application, obtained by means of electrodeposition and solvothermal synthesis.

Andrea Giaccherini

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"
MATERIAL SCIENCE, PHYSICAL CHEMISTRY-CHEMICAL PHYSICS, SPECTROSCOPY

Chalcogenides such as CdSe and CdTe thin-films are well known semiconductors, used in manufacturing of last generation photovoltaic components. Toxicity and shortage of the involved elements must be considered in the advancement of technology. Hence scientific community is focusing attention on new compounds based on economic and low-environmental impact elements such as Cu, Sn, Fe and Zn. In particular, quaternary semiconducting materials based on the kesterite ($\text{Cu}_2\text{ZnSnS}_4$) mineral structure are the most promising candidates to overtake the current generation of light-absorbing materials for thin-film solar cells. Among many different synthetic strategies, my work focus on the optical and structural characterization of the products obtained by means of two different synthetic strategies, electrodeposition and solvothermal synthesis. Electrodeposition is known as a low-cost semiconductor growth technique for applications in electronic devices. Surface limited electrodeposition of atomic layers, can be performed exploiting their underpotential deposition by Electrochemical Atomic Layer Deposition (E-ALD) technique to obtain sulphides thin films. Solvothermal synthesis is a method for preparing a variety of materials, with different geometries and morphologies, under moderate to high pressure and temperature that facilitates the interaction of the precursors, the process allows the facile synthesis of sulphides nanoparticles.

Poster

Ciclo XXX

Laboratory tests about resistivity variation in soil, in connection with root rate and soil humidity and bulk density

Yamuna Giambastiani

DOTTORATO IN GESTIONE SOSTENIBILE DELLE RISORSE AGRARIE, FORESTALI E ALIMENTARI - Ingegneria Agro-Forestale (IAF) - Dipartimento dei Gestione Sistemi Agrari, Alimentari e Forestali (GESAAF)

FORESTRY, GEOPHYSICS, BIOSYSTEM

Knowledge about root system distribution covers an important role in slope shallow stability studies, as this factor grants an increase in soil geotechnical properties and determines a different underground water circulation. Published studies about in situ application of ERT (Electrical Resistivity Tomography) analysis show how the root presence affects the measurable soil resistivity values, confirming the suitability to investigate the application of such technique, aiming to estimate root density in soil with an indirect and non-invasive method. This study, laboratory-based and led on reconstructed samples in controlled condition, aim to find a correlation between the resistivity variations and the various factors that can affect them (humidity, bulk density, presence of foreign bodies, temperature). Root presence is simulated inserting bamboo spits. The tests are repeated in time, monitoring the natural variations in humidity (evapotranspiration) and bulk density (compaction). The first results show an increase of resistivity with the decrease of mean humidity that follows a potential trend; data measured in the spitted sample can be statistically considered as a different population in respect to the data from the bare earth sample, giving credit to the hypothesis that the wooden spit presence could be indirectly quantified from geoelectric data. Additional tests are currently underway.

Poster

Ciclo XXX

Size distribution and Rare Earth Elements
determination in arctic aerosol

Fabio Giardi

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

ANALYTICAL CHEMISTRY, ENVIRONMENTAL / POLLUTION

The aerosol is one of the most important forcing factors, affecting the polar regions and the climate in general, but its contribution on the climate is still uncertain. To better understand the role of the atmospheric particulate in polar regions, my project is focused on the development of a suitable method to analyze Rare Earth Elements and other Heavy Metals through Inductively Coupled Plasma Mass Spectrometry (ICP-MS) and the further analysis of samples collected in the Arctic. The analysis of these elements, supported by the size distribution of the particles, are useful to identify the source and origin region of the aerosol. The results could allow to estimate the weight of every source and, in particular, the contribution of anthropic activities from industrialized areas.

Poster

Ciclo XXIX

Photosynthesizing on metal excess: copper differently induced changes in various photosynthetic parameters in copper tolerant and sensitive *Silene paradoxa* L. populations

Elisabetta Giorni

DOTTORATO IN BIOLOGIA - Biologia Vegetale - Dipartimento di Biologia (BIO)

ECOLOGY / ETHOLOGY / EVOLUTION, PLANT PHYSIOLOGY

This work investigated copper-induced changes in photosynthetic activity in two contrasting populations of *Silene paradoxa* L. A metallicolous Cu-tolerant population and a non metallicolous one were grown in hydroponic culture and exposed to different copper sulphate concentrations for different times. Copper accumulation and several photosynthetic parameters were measured to assess different effects of copper exposure on plants from the two populations. The Cu-tolerant population showed a more efficient ability to photosynthesize in the presence of copper excess. Copper-imposed limitations were present not only at a different degree, but also of different nature in the two populations. In the tolerant population, the most limiting factor to photosynthesis seemed to be copper-imposed stomatal closure whereas copper-mediated biochemical limitation was scarce and copper-mediated reduction in mesophyll conductance almost non-existent. In the sensitive population, copper largely affected all the parameters, so that its photosynthetic activity experienced any kind of limitations, diffusional and especially biochemical. The lower copper concentrations accumulated in the tolerant plant could be one of the factor concurring to the reported differences in photosynthetic activity, but also a higher capacity of internal detoxification and compartmentalization of the metal could not be excluded.

Poster

Ciclo XXX

Multimodal nonlinear microscopy applied to the study of tissue lesions

Cristina GiubaniINTERNATIONAL DOCTORATE IN ATOMIC AND MOLECULAR PHOTONICS -
Laboratorio Europeo di Spettroscopie non Lineari (LENS)

MICROSCOPY, OPTICS AND PHOTONICS, BIOPHYSICS

Modern nonlinear microscopy techniques offer promising label-free solutions to improve diagnostic performances on tissues, giving a high-resolution label-free alternative to histological examination of tissues. These techniques provide not only tissue morphology information but also about its functions. We have tested and compared the morphology of collagen in the connective tissue within cutaneous samples containing melanocytic lesions of different degrees of invasiveness. As the collagen fibers produces a high SHG signal, exploitable for imaging of the same collagen within the dermis, coupling TPEF and SHG to fluorescence-lifetime imaging microscopy (FLIM) allows to get more information on the molecular microenvironment of a fluorescent molecule or its energy exchanges. Moreover, through collagen fibers organization and their architectural and structural geometry it can be determined how these factors affect the proliferation of a lesion within the tissue. This study aims to characterize the morphology of collagen in healthy and pathological tissues in order to understand the different structural and functional organization of the collagen fibers within these tissues. Identifying the organization of the collagen fibers around the lesional regions, we can also understand the role of such architecture within the process of invasion, as well as to characterize the morphology of the tissue itself.

Poster

Ciclo XXIX

Self-assembly, stability and performances of water-based cleaning systems

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SURFACE SCIENCE, PHYSICAL CHEMISTRY-CHEMICAL PHYSICS, FLUID DYNAMICS,
POLYMER SCIENCE

Cleaning is crucial to many different applications, ranging from detergency processes in laundry and hand-washing applications to the removal of detrimental films from solid substrates. Water-based systems for cleaning typically consist of dispersions in water of surface-active agents and other additives. This project aims at identifying those parameters based on surfactant composition and structure that could be correlated to the stability and properties of the cleaning systems. Furthermore, a model able to predict the self-assembly and performances of water-based cleaning systems will be developed.

Poster

Ciclo XXIX

A study on well integrity in a natural analogue for the geological CO₂ storage

Ana Hernandez-Rodriguez

DOTTORATO IN SCIENZE DELLA TERRA - Dipartimento di Scienze della Terra (DST)

MATERIAL SCIENCE, COMPUTATIONAL MODELING, STATISTICAL MECHANICS -
THERMODYNAMICS, ENVIRONMENTAL / POLLUTION, GEOCHEMISTRY AND
VOLCANOLOGY, MINERALOGY AND PETROLOGY

This study presents the results obtained so far through a study on well integrity in a natural analogue for the geological storage of CO₂. Both a spa and a CO₂ production plant are present in the site of interest, which is situated in Southern Tuscany. The diffuse CO₂ flux from soil was measured by means of the accumulation chamber method in selected zones of the study area, to assess the natural CO₂ leakage through the soil. The measured CO₂ flux data were partitioned in different populations and mapped. Merging the obtained data with those from previous studies, it was possible to estimate a total diffuse output of deep CO₂ in 48.7 tons per day with an error of 8.1 tons per day from an area of 7400 m². Reactive Transport Modelling was used to investigate the integrity of an ideal well for CO₂ exploitation with Portland-type cementing material by means of the software package TOUGHREACT v2.1. The elements involved in the model are: carbonate host rocks, Portland cement, stainless steel casing, and fluids flowing in the borehole, constituted by CO₂ and water. Measured CO₂ flux data were used to constrain CO₂ saturation in the soil.

Poster

Ciclo XXX

Isoxazol-5-(2H)-one derivatives as human neutrophil elastase (HNE) inhibitors

Antonella Iacovone

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ORGANIC CHEMISTRY, DRUGS-HEALTH

Human neutrophil elastase (HNE) is an enzyme belonging to the family of serine protease. It is a small, basic and soluble glycoprotein of about 30 kD and it is stored in azurophilic granules of polymorphonuclear neutrophils. It is involved in a variety of activities, such as degradation of the structural proteins of extracellular matrix, protection of the organism from pathogens and regulation of the inflammatory processes. HNE performs its proteolytic action through the catalytic triad consisting of Ser195-Asp102-His57, more specifically the OH group of the serine attacks the carbonyl carbon of the substrate leading to the breaking of the amide bond. In physiological conditions, the action of HNE is regulated by its endogenous inhibitors (α -1-PI, α -2 macroglobulin, SLPI and elafin). If the balance between proteases and antiproteases disappears, the excess of HNE activity can cause tissue damage. Among the respiratory system pathologies associated with increased HNE are COPD, CF, ALI and ARDS, but also for rheumatoid arthritis, atherosclerosis and cancer an involvement of HNE was demonstrated. The research performed in this first period as PhD student consisted in the synthesis of new potential HNE inhibitors with isoxazol-5(2H)-onic scaffold.

Poster

Ciclo XXVIII

Semi-synthetic strategy to obtain aberrantly
N-glycosylated Myelin Oligodendrocyte Glycoprotein
as a specific autoantigen of multiple sclerosis

Matthaia Ieronymaki

DOCTORATE IN CHEMICAL SCIENCES (UNIVERSITY OF CERGY-PONTOISE) -
Dipartimento di Neuroscienze, Psicologia, Area del Farmaco e Salute del Bambino
(NEUROFARBA)

ORGANIC CHEMISTRY, DRUGS-HEALTH, PHARMACOLOGY, CELLULAR BIOLOGY,
RECOMBINANT PROTEINS

Multiple sclerosis (MS) is one of the most known inflammatory and demyelinating diseases of the central nervous system (CNS) with unknown etiology. It is widely believed that antibody-mediated mechanisms are involved in the pathogenesis of at least a subset of patients with CNS inflammation. Multiple types of autoantibodies can be present in sera of MS patients and if these autoantibodies are specific for the disease, they can be used as diagnostic or prognostic biomarkers. Our research group has previously demonstrated that an aberrant N-glycosylation in a designed β -turn peptide structure is able to detect specific autoantibodies in an MS patients' population. Moreover, Myelin Oligodendrocyte Glycoprotein (MOG) that is expressed in the outermost surface of myelin sheath, is considered to be a putative MS auto-antigen even if its role is still a matter of debate. In this context, we hypothesize that aberrant N-glycosylation of Asn31, native glycosylation site of hMOG, is involved in the etiopathogenesis of MS. By a Native Chemical Ligation approach we are developing a semi-synthetic strategy to obtain the N-glycosylated hMOG1-117 forming an amide bond between Asn31(Glc)hMOG(1-34) coupled to a 4-sulfamylbutyryl linker (synthesized by SPPS) and the recombinant protein hMOG(35-117) bearing an N-terminal cysteine and expressed in *E. coli*.

Poster

Ciclo XXX

Bindi's grapevine model implementation: phenology, biomass partitioning and nitrogen balance

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AGRICULTURE

Grapevine simulation models have become useful tools for estimating grapevine yield and quality in present and future climatic conditions. According to this, Bindi et al. (1997) introduced a simple process-based model in order to describe grape development, growth and yield taking into account water stress conditions. In this way, the main objective of this project is the implementation of Bindi's model with new aspects of phenology and biomass partitioning, as well as the introduction of nitrogen balance. Additionally, the project will consider the variability in quantity and quality production when extreme events take place. The expected results should predict better Bindi's model responses on grapevine yield and quality through the implementation of these processes. For instance, the plant phenology may be improved by introducing dormancy and post-dormancy phase. These latter, should be considered fundamental for a more accurate bud break date estimation. Moreover, for understanding the biomass allocation among different plant organs, the partitioning will be implemented. Finally, nitrogen balance may be introduced for testing effects on grapevine yield and quality. In conclusion, the implementation of Bindi's model should be useful to provide a more accurate approach for evaluating grapevine quantity and quality production in present and future climatic scenarios.

Poster

Ciclo XXIX

Non-SELEX: a valuable tool for aptamer selection.
The case of tau protein.

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ANALYTICAL CHEMISTRY, NEUROSCIENCE

Aptamers are short single stranded oligonucleotides that have been presented to rival antibodies for many applications. After aptamers development in 1990 several methodologies have been applied to their selection. Selection is usually realized by SELEX (Systematic Evolution of Ligands by EXponential enrichment) which needs usually 10-15 rounds to be accomplished. Here we presents preliminary results of Non-SELEX method applied to the selection of DNA aptamer for tau protein, one of validated biomarker for Alzheimer's disease early diagnosis. The novel bioreceptor, once characterized, will hopefully give more opportunities to integrate existing and novel platforms for AD diagnosis.

Poster

Ciclo XXIX

Effect of different agricultural management on ants community in organic and non organic vineyards

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ECOLOGY / ETHOLOGY / EVOLUTION, AGRICULTURE

In the cultivation of grapevine (*Vitis vinifera*) several management methods are employed, from organic production to intensive conventional farming. In this highly managed ecosystem ants, which may be both pests and pest-control agents at the same time, often represent a large fraction of insect biomass. Ant assemblages often reflect the degree of habitat disturbance, degradation, and may also be used as indicators of biodiversity loss in other taxa. This study investigates how different management options used in vineyards affect ant assemblages. Ten vineyards were selected in the Chianti area near Florence; five of these were managed following conventional protocols (allowing the use of agrochemicals) while five followed organic farming principles. Ants were sampled using pitfall traps during the summer 2014. More than 4000 ants were sampled, representing 19 species. The vineyards under organic management showed greater species density, even though the same species were found in both the types of vineyards. Multivariate analysis confirmed the difference in the structure of these assemblages. The results suggest that pesticide application adversely affected ant diversity and that the effect of insecticide application is greater than that of herbicides. These results agree with the idea that conventionally managed agroecosystems, where intensive use of agrochemicals is made, may undergo an impoverishment of their arthropod fauna.

Poster

Ciclo XXX

The redox-dependent folding state of human Cox17 visualized by in-cell NMR

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CELLULAR BIOLOGY

In-cell NMR spectroscopy was established as a method to investigate biological macromolecules in their physiological environment at atomic resolution. In our work, we applied this technique to study folding and redox state of the human mitochondrial protein Cox17 in the cytoplasm of human cells. Cox17 is a metallochaperone involved in the delivery of copper ions to the cytochrome c oxidase. Cox17 contains six conserved cysteines, of which four can form two structural disulfide bonds and two act as the binding site for copper. Cox17 exists in three oxidation states depending on the disulphide bonds formation: fully reduced, partially oxidized and fully oxidized. Cox17, synthesized in the cytoplasm in the reduced unfolded state, is imported inside the IMS undergoing an oxidative folding and reaching its functional partially oxidized form. Transient expression of human Cox17 was performed in human cells. Cox17 localization was mainly cytoplasmic and its folding was monitored through NMR experiments: Cox17 is mainly folded, in a conformation unable to translocate inside the IMS. Cox17 was co-expressed together with a cytoplasmic thiol-disulfide regulating protein. Our findings highlights that in living cells the folding and the redox state of hCox17 before its import inside the IMS is modulated by specific partner.

Poster

Ciclo XXX

Predictive modelling for dairy cow welfare assessment

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COMPUTATIONAL MODELING, BIOINFORMATICS, ANIMAL SCIENCE

Dairy cow welfare is a fundamental aspect in modern breeding system, being one of the most incisive factors affecting a farm, both from economic and health point of view. Despite of its importance, animal welfare is still difficult to assess properly. Objective parameters for animal welfare assessment are often tied to both single animal and herd healthiness: presence of various diseases in a farm is, for example, one of these parameters; it is, however, difficult to identify direct connections between these parameters. One helping hand comes from Information Technology (IT): the so-called statistical learning theory. Starting from raw data, computer algorithms are able to understand the structure underlying them and to elaborate it into a model representing all the relations between data. Aim of the project is to analyze data from an experimental farm about both lactation (data automatically recorded by modern robotic milking systems during and after each milking) and health status, therefore elaborating predictive models able to predict dairy cow welfare when applied to new data coming from different farms. Various statistical algorithms will be tested to assess which one fits best to our data.

Poster

Ciclo XXX

Antimicrobial activity of Auranofin

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DRUGS-HEALTH, PHARMACOLOGY

Bacterial resistance is a rapidly escalating threat to public health and highly relevant is the need to find new molecules to treat bacterial infection. However, developing a new drug is highly expensive and time consuming and the rate of success is very low. The use of drug repurposing is more affordable and achievable strategy than novel drug discovery. My PhD program is focusing on the testing of the antimicrobial activity of Auranofin, a drug approved to the treatment of reumatoid arthritis. We will apply different screening methods, on a wide panel of human pathogenic bacteria, as the disk diffusion test and microplate assays to determine the overall effect, the values of the minimal inhibitory concentration (MIC) and minimal bactericidal concentration (MBC). Moreover, by the use of the disk diffusion assay mutants will be searched, which could then used to understand, through the comprehension of the resistance mechanisms, the Auranofin molecular targets in bacterial cells, which may ultimately help to design new drug derivatives with increased antibacterial activity.

Poster

Ciclo XXVII

Improving thermal performance of earth-to-air heat
exchanger by wetting the ground: an experience in
Southern Iraq

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DOTTORATO IN GESTIONE SOSTENIBILE DELLE RISORSE AGRARIE, FORESTALI E
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ENERGY ENGINEERING, ENVIRONMENT, RESOURCES AND SECURITY

Earth to air heat exchangers (EAHE) can reduce energy consumption required for heating and cooling of buildings. The aim of this study was to compare thermal performance of EAHE in dry and artificially wetted soil. Two experimental EAHE were built and tested from June 2013 till September 2013. Both systems consisted in a single PVC pipe buried at a depth of 2 m. Soil around one exchanger was wetted by a drip tubing placed 10 cm above the air pipe. To better evaluate the air conditioning performance of EAHE two separated period were considered, one in the hottest part of the day 12:00 am, 4:00 pm and one in the colder part 2:00 am, 6:00 am. Considering only the hottest part of the day, on average, the difference between outlet and inlet air temperature was lower for WE -7.60°C than for DE -6.32°C . In the colder period the difference between outlet and inlet air temperature was higher for WE $+3.82^{\circ}\text{C}$ than for DE $+3.14^{\circ}\text{C}$. Results indicated that wetting the soil around EAHE can improve the heat exchange efficiency.

Poster

Ciclo XXX

The click chemistry approach for the development of
selective carbonic anhydrase inhibitors

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ORGANIC CHEMISTRY, DRUGS-HEALTH

The development of selective modulators of the carbonic anhydrase enzymes (CA, EC 4.2.1.1) represents the key approach for the identification of new and promising drugs useful for the treatment of various diseases such as the glaucoma, Alzheimer, obesity and obesity-related pathologies, cancer and infections. Herein we report the use of the click chemistry approach as efficient tool for the synthesis of selective inhibitors against the human CAs.

Poster

Ciclo XXX

Multivariate approach for screening and optimization
of RP-UPLC method performance for a formulated
vaccine.

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ORGANIC CHEMISTRY, ANALYTICAL CHEMISTRY, PHYSICAL CHEMISTRY-CHEMICAL
PHYSICS, SPECTROSCOPY, POLYMER SCIENCE, BIOPHYSICS, BIOINFORMATICS,
RECOMBINANT PROTEINS, VACCINES; GLICOCONJUGATES

The application of QbD principles to analytical method development is focused on the concept to build quality during method development. For this reason, the methods to be developed had to satisfy requirements described in Analytical Target Profile (ATP). In particular, the resulting methods have to satisfy: i) minimum requirements related to method performance (precision, sensitivity, accuracy, selectivity, etc) and ii) minimum requirements related to assay feasibility that is applicability to a routine Quality Control testing. Recombinant proteins are the active components of the Meningococcal Vaccine and the control of method variables is important to assure the RP-UPLC assay quality. For this reason, preliminary screening studies of two critical factors, identified in vials type and antigens concentration, were performed to select the best operative conditions and ensure Sensibility and Repeatability of the method. Asymmetric screening matrices (based on Free-Wilson model) were set-up to study the two factors. The software used for experimental plans construction was NEMRODW[®]2015. The graphic effects study of the single variables and their interactions allowed identifying the optimum operative conditions.

Poster

Ciclo XXVII

Self-folding microstructures with active liquid crystalline part

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MATERIAL SCIENCE, OPTICS AND PHOTONICS, APPLIED PHYSICS, ROBOTICS

Liquid crystalline elastomers (LCEs) are soft materials, that can respond to the external stimuli such as light and temperature. They combine properties of liquid crystals (LCs) and polymer networks. Creating different alignment in LCEs is possible, and allows for several types of actuation of the microstructure. Thin film LCE structures capable of self-folding into complex 3D configurations have been investigated in micro scale for application in such area as drug delivery. Combining two types of polymers – active (LCE) and passive (commercial photo resist), it is possible to create small elastomer devices that exploit bending mechanism. One of the examples is a reflective grating that can change its position with respect to the incident beam. A LCE micro-box is fabricated to demonstrate the self-folding concept. Vertical alignment available in laser written compounded structures, allow for realization of more complex 3D deformability and configuration. Applications can be envisioned, for instance, in tunable complex photonic devices and drug delivery/medical diagnostics.

Poster

Ciclo XXIX

Generating solitons on discrete Heisenberg chains and how to manipulate qubits with them

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THEORETICAL PHYSICS, COMPUTATIONAL MODELING, MATTER PHYSICS

Solitons are non-linear excitations with specific space and time localization; they propagate along one-dimensional media with constant shape and velocity, and are further characterised by stability against noise and perturbations. These features make them particularly suitable for some practical applications, such as the transmission of signals between distant parties. A magnetic soliton on a spin chain could be used, for example, to reach and control the state of a qubit locally coupled to the chain, giving the advantage of addressing a single target without disturbing its environment, which is a puzzling problem in solid-state quantum computer proposals. In view of the possible use of solitons as a means for qubit manipulation, a practical scheme to achieve the generation of soliton-like excitations on discrete classical Heisenberg chains, by the application of a time-dependent magnetic field on one chain end, is proposed. A theoretical model describing the dynamics of the qubit density matrix subjected to soliton transit is also presented. Both models have been tested via numerical simulations and results here discussed.

Poster

Ciclo XXIX

Cancer stem cells in osteosarcoma

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CELLULAR BIOLOGY, ONCOLOGY, STEM CELLS

Osteosarcoma (OS) is the most common primary bone tumor. Most of OS which occur in children and young adults are high grade and usually these develop in the metaphysis of the long bones. The current management of this cancer is the surgical excision in association with chemotherapy, which may be followed by radiation therapy. Despite this multi-modal therapy the outcome remains poor. An innovative prospect for the battle against OS emerged from studies which highlight a key role of cancer stem cells (CSCs) in the development, maintenance, chemoresistance, and relapse of cancers, indicating these undifferentiated transformed stem-like cells as possible primary targets for more effective anti-cancer therapies. CSCs present surface markers typical of mesenchymal stem cells (MSCs) and express marker genes typical of embryonic stem cells (ESCs). This is a possible explanation as to why therapy seems to be initially effective, but the patient later relapses because the subset of CSCs was not completely eradicated. In order to identify possible molecular targets for a specific therapy against OS, we have established primary cell cultures from human high grade OS biopsies collected. We have isolated CSCs from the primary cell cultures of OS (OS-CSCs) and evaluated their stemness.

Poster

Ciclo XXX

A theory of River Restoration through mitigation of hydrogeological risk

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URBAN DESIGN, AGRICULTURE, FORESTRY, NATURAL HAZARDS, GEOLOGY AND
TECTONOPHYSICS, HYDROLOGY

The hydrogeological emergency is on the agenda, both on a national and local level, not only because of the special characteristics of our peninsula, but also because of bad management of specific local climatic and environmental features on the part of related local institutions. This situation, in light of the relative immaturity of the main related disciplines often creates uncertainty in the work done on the subject, with consequences for natural and human systems. From the point of view of land-planning for the riparian areas and of the River Restoration, three main operational proposals have been identified: to preserve (e.g., through a meticulous attention to maintenance of the underlying systems of the river banks); to limit (e.g., integrating the measures already taken in the area with functional enhancements); to restore (e.g., with a multidisciplinary approach that allows a combination of geological and engineering measures with landscape restoration). These recommendations are recalibrated as needed depending on the specific stretch of river at issue for intervention. At the same time a coordination is necessary in order not to lose sight of the whole picture, involving not only institutions but also local communities in territory monitoring operations.

Poster

Ciclo XXVIII

Development of innovative systems for cleaning and protection of Cu-based metallic artifacts

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PHYSICAL CHEMISTRY-CHEMICAL PHYSICS, CULTURAL HERITAGE PRESERVATION,
POLYMER SCIENCE

The aim of the PhD project is to supply new materials and methods to clean and protect ancient metallic artifacts. The research activity concerns innovative cleaning materials for copper-based alloys consisting of a physical gel-complexing agent system. The gel formulation was inspired by cosmetics, in particular by those beauty peelable masks used to remove impurities from skin, mainly made of poly(vinyl)alcohol (PVA). The addition of a complexing agent for Cu^{2+} , such as Rochelle Salt, EDTA or polyamines allows the selective removal of corrosion products, maintaining the "noble patina" of cuprite (Cu^+) intact. The cleaning system is applied as a viscous solution and after few hours it can be easily peeled off as a film from the surface, thanks to the evaporation of the volatile fraction. Some advantages of these systems are: i) improved chemical cleaning control than commonly used restoration methods; ii) application on rough and irregular surfaces thanks to the initial fluency; iii) application on delimited areas without any diffusion in the adjacent zones; iv) modulation of gel viscosity depending on the application surfaces; v) simultaneous mechanical and chemical action to improve cleaning performances; vi) transparency of the gels; vii) vehiculation of more effective complexing agents.

Poster

Ciclo XXVIII

Mimicking serin protease inhibitor H1 chaperone
function in collagen biosynthetic pathway via the
template assembled synthetic protein approach

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ORGANIC CHEMISTRY, DRUGS-HEALTH, PHARMACOLOGY, BIOINFORMATICS

Collagen superfamily comprises twenty-eight collagen types involved in a broad range of functions, whose molecular hallmarks are the multiple repetition of the Gly-X-Y motif and the unique triple helical structure.

The 47 kDa SERPIN Hsp47 plays a key role in collagen superhelix folding process, selectively recognizing and transferring procollagen molecules from the ER to the Golgi apparatus.

We are proposing a TASP as an innovative pharmacological tool to explore Hsp47 actual impact on collagen turnover, with the purpose to investigate its role in collagen-related diseases. According to the TASP approach, an appropriate scaffold should act as a built-in device for peptide blocks suitably selected from the functional part of Hsp47, mimicking the native folding of the protein chain.

Therefore, with the support of molecular modelling techniques, we designed a small library of TASP candidates, and we selected the most promising molecule either in terms of RMSD values, or in terms of docking energy estimations.

The synthesis of the selected TASP is currently on going and will be followed by *in vitro* biological activity evaluation, considering both its collagen binding ability and fluctuations in collagen production induced in cultured Normal Human Dermal Fibroblasts.

Poster

Ciclo XXX

Vibrational landscape on the nest of *Polistes dominula*

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ECOLOGY / ETHOLOGY / EVOLUTION, ENTOMOLOGY

Vibrations carried in the substrate are considered a very old and ubiquitous communication channel. The paper nest of *Polistes* wasps favors the transmission of vibratory signals and indeed several behaviors performed by wasps on nest produce vibrational signals. The aim of our work was to describe the vibrations produced by the wasp *Polistes dominula* on nest, in order to understand their putative role in the communication system of this species. We recorded substrate-borne vibrations with a laser vibrometer connected to a video camera pointed at the nest. First we focused on abdominal wagging (AW), a behavior performed by female that consists in horizontal abdomen oscillations. We found significant individual differences in the various parameters (e.g. dominant frequency and Pulse Repetition Time) that characterize AW. In order to verify the dependence of the feeding contest in affecting AW to vary nutritional state of the larvae we compare AW features during normal breeding and nutrition contexts right after larval starvation. We found a significant, even if limited, difference in some parameters of AW between the different conditions. Our preliminary results show that AW may be involved in the adult-larvae communication. Further studies should be however performed to fully support this hypothesis.

Poster

Ciclo XXVIII

The diagnostic boundary between autism spectrum disorder, intellectual developmental disorder and schizophrenia spectrum disorders

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NEUROSCIENCE

During the last ten years the prevalence of autism and Autism Spectrum Disorder (ASD) have increased greatly. In the 60s the most reported rate was 0.5/1.000, while currently the prevalence of ASD in adults is 1/100. Such increase in prevalence estimates raises a number of questions as to the origins of this increase. A recurring issue is the boundaries between ASD, Intellectual Developmental Disorder (IDD) and Schizophrenia Spectrum Disorders (SSD). In clinical practice many people with IDD have both autistic traits and a concurrent diagnoses of SSD, and many with ASD have coexisting IDD and receive a diagnosis of SSD. Furthermore people with SSD may often have a mild IDD or other cognitive problems prior the onset of psychotic disorder. Recently evidences regarding protein alterations regulating synapses growth in Central Nervous System seems to suggest that IDD, ASD and SSD are part of a single group of neurodevelopmental disorders. The aim of the research project is to define the core symptoms and overlapping clinical characteristics of IDD, ASD and SSD to contribute to the development of better diagnostic criteria. A systematic mapping of the literature on the research topic was conducted. Contemporarily, an experimental search was started.

Poster

Ciclo XXX

Genome-scale metabolic reconstruction of
Acinetobacter baumannii species

Luana Presta

DOTTORATO IN BIOLOGIA - Genetica e Microbiologia - Dipartimento di Biologia
(BIO)

COMPUTATIONAL MODELING, BIOINFORMATICS, METABOLOMICS

Genome-scale metabolic reconstructions are a powerful tool that allow a system-level analysis of organisms, based on simple genome annotation data and biochemical knowledge from literatures and databases. This approach, used on multiple strains of a species, can help to define the metabolic essence of a microbial species and to delineate growth differences that correlate with the adaptation process to a particular microenvironment. Hence genome-scale metabolic model reconstruction of the whole *Acinetobacter baumannii* species has been carried on. *A. baumannii* recently emerged as a new clinical threat to human health, particularly in nosocomial environment. Current lack of effective clinical solutions to treat this pathogen reflects the necessity to carry out systems-level studies that could contribute to the development of an effective therapy.

Poster

Ciclo XXIX

Partition functions and stability criteria of topological insulators with non-Abelian edge excitations

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DOTTORATO IN FISICA E ASTRONOMIA - Fisica - Dipartimento di Fisica e Astronomia

THEORETICAL PHYSICS, MATTER PHYSICS

The study of topological phases of matter has considerably grown in recent years and new systems have been investigated both theoretically and experimentally in several spatial dimensions. These phases, e.g. the Quantum Spin Hall Effect, Topological Insulators and Topological Superconductors have some features similar to the Quantum Hall Effect but do not require magnetic fields. I will focus on two-dimensional time-reversal invariant Topological Insulators, modeled by pairs of quantum Hall states carrying opposite spin and chirality. I will describe the edge excitations of general Abelian and some non-Abelian states by means of their partition function. I will focus on the problem of the stability of topological phases protected by time-reversal symmetry and I will show how this is related with the existence of a discrete Z_2 anomaly and the lack of modular invariance of the partition function. In the absence of the anomaly, for general Abelian systems exists a set of interactions, allowed by time reversal symmetry, that can gap completely the system and make it topologically trivial. I will show how the same argument holds for systems with non-Abelian edge excitations, and I will give the form of the time-reversal invariant interactions that completely gap the systems.

Poster

Ciclo XXIX

DNA technology for small molecules sensing: a new approach for acetamiprid detection

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DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

ANALYTICAL CHEMISTRY, ENVIRONMENTAL / POLLUTION, ELECTROCHEMISTRY

Pesticides detection remains a challenge: chromatographic methods are traditionally used due to their sensitivity, reliability and efficiency, but they are time-consuming and require trained technicians. Over the last few years, considerable attention has been given to the development of biosensors as an alternative for pesticides detection, and DNA-based sensors are one of the most representative examples for environmental field monitoring. An electrochemical DNA array for Acetamiprid, a neonicotinoid insecticide, is presented: it is based on a dual signal strategy, employing a polyaniline film and gold nanoparticles as sensor platform and an enzyme-linked label for sensitive detection. Polyaniline film and gold nanoparticles were grown on graphite screen-printed electrodes surfaces via electro-polymerization and electrochemical deposition, respectively. The polyaniline-gold nanostructured sensors were modified with a mixed monolayer of a thiol-tethered DNA aptamer and a spacer thiol. The aptasensor was able to capture the pesticide from the sample solutions. An enzyme-amplified detection scheme, based on the coupling of a streptavidin-alkaline phosphatase conjugate and biotinylated secondary aptamer was then applied. The enzymatic product was detected using differential pulse voltammetry. Experimental parameters of the realized DNA-based sensor were optimized using optical and electrochemical techniques, obtaining preliminary results measuring different concentrations of Acetamiprid in water samples.

Poster

Ciclo XXIX

Core-shell nanoparticles for DNA delivery actuated by magnetic fields

Annalisa Salvatore

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DRUGS-HEALTH, PHARMACOLOGY, NANOMEDICINE, NANOPARTICLES

One of the major areas of research in nanomedicine is the design of drug delivery systems with remotely controllable release of the drug. Despite the enormous progress in the field, this aspect still poses a challenge, especially in terms of selectivity and possible harmful interactions with biological components other than the target. We report an innovative approach for the controlled release of DNA, based on clusters of core-shell magnetic nanoparticles. The coating of magnetic nanoparticles with an inert shell, such as gold, has been proposed in order to add further properties (enhance biocompatibility, protection of the magnetic core against oxidation) to the nanoparticles, without modifying their superparamagnetic behaviour. We have accomplished the conjugation of Au@Fe₃O₄ with a thiolated single-stranded oligonucleotide, whose pairing with a half-complementary strand in solution induces clusterization. The application of a low frequency (6 kHz) alternating magnetic field induces DNA melting with the release of the single strand that induces clusterization. The release and delivery of the staple is based on the hyperthermic heating of clusters of DNA coated magnetic NPs. The possibility of steering and localizing the magnetic nanoparticles, and magnetically actuating the DNA release discloses new perspectives in the field of nucleic-acid based therapy.

Poster

Ciclo XXX

Early environmental therapy rescues brain development in a mouse model of Down Syndrome

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DRUGS-HEALTH, NEUROSCIENCE

Down syndrome (DS), the most common genetic disorder associated with mental retardation, is an untreatable condition characterized by a number of developmental defects and permanent deficits in the adulthood. Ts65Dn mice, the major animal model for DS, display severe cognitive and synaptic plasticity defects closely resembling the human phenotype. Here we employed a multidisciplinary approach to investigate, for the first time in developing Ts65Dn mice, the effects elicited by early environmental enrichment (EE) on cognitive abilities, hippocampal synaptic plasticity, visual function maturation, GABAergic inhibition and brain-derived neurotrophic factor. We report that exposure to EE results in a robust increase in maternal care levels received by pups, increased BDNF expression and normalization of visual acuity development, hippocampal long-term potentiation, object-recognition memory and GABA vesicular synaptic transport. These findings highlight the beneficial impact of early environmental stimuli and their potential for application in the treatment of major functional deficits in children with DS.

Poster

Ciclo XXX

Anion complexes with tetraazine-based ligands

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INORGANIC CHEMISTRY, SUPRAMOLECULAR CHEMISTRY

Supramolecular chemistry is "the chemistry of the non-covalent bond" or "the chemistry beyond the molecule". According to these definitions, the focus of this discipline lies on chemical system formed by a number of discrete molecular subunits held together in a supramolecular adduct by non-covalent forces.

Anion coordination chemistry, a maturing aspect of supramolecular chemistry, dedicates itself to the binding of anionic species with suitable receptors and to the study of the resulting complexes. Among other well-established non-covalent forces, the so-called "anion- π interactions", the interactions between aromatic systems and anions, have been recently recognized as an important factor in the formation and stability of anion complexes.

Here we present our ongoing study onto the coordination properties towards several anions of a family of symmetrical 3,6 N-alkyl morpholine-disostituted 1,2,4,5 tetraazines, namely the N-methylenic and the N-ethylenic ones. The study has been performed on selected anions focusing onto the thermodynamic and structural aspects of the coordination using several techniques: equilibrium constants for ligand protonation and anion complex formation were determined by means of potentiometric titrations in aqueous media, thermodynamic data were obtained through isothermal titration calorimetry and structural information about the complexes was gained by means of single-crystal X-ray diffraction.

Poster

Ciclo XXIX

High-pressure chemistry in nanoconfined systems:
polyCO and 1D-PolyAcetylene/Zeolites
nanocomposites

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MATERIAL SCIENCE, PHYSICAL CHEMISTRY-CHEMICAL PHYSICS, SPECTROSCOPY

High-pressure polymerization of simple molecules in the subnanometric pores of silicalite, a 3D pure SiO_2 zeolite, can be exploited to produce novel nanocomposite materials, recoverable at ambient P, with remarkable mechanical, electrical and optical properties. Compared to the high-pressure polymerization in the bulk phase of the pure starting molecule, the extreme confinement conditions allow to synthesize extended single polymeric chains with conformational stereoselectivity and stabilize them at ambient conditions against atmospheric degradation. Recently, materials such as PE-SIL (PolyEthylene SILicalite) or PASIL (PolyAcetylene SILicalite) have been synthesized this way. Here are presented our last results about the high-pressure polymerization of CO and acetylene inside 3D and 1D nanochannels of silicalite. In particular the interest in the polyCO/zeolite nanocomposite is related to the potential applications as high energy density material. Switching from 3D to 1D pure silica zeolite hosts (ZSM-22) allows to obtain even more interesting results. The high-pressure polymerization of acetylene inside ZSM-22 gives rise to the formation of conducting PolyAcetylene (PA) chains along the 1D host channels of ZSM-22. In this system, the electronic density of states of PA is expected to exhibit van Hove singularities related to quantum 1D confinement, which could lead to future technological exploitations.

Poster

Ciclo XXX

A generalized sense of number

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Area del Farmaco e Salute del Bambino (NEUROFARBA)

NEUROSCIENCE, PSYCHOLOGY

Much evidence has accumulated to suggest that many animals, including young human infants, possess an abstract sense of approximate quantity, a number sense. Most research has concentrated on apparent numerosity of spatial arrays of dots or other objects, but a truly abstract sense of number should be capable of encoding the numerosity of any set of discrete elements, however displayed and in whatever sensory modality. Here, we use the psychophysical technique of adaptation to study the sense of number for serially presented items. We show that numerosity of both auditory, visual and tactile sequences is greatly affected by prior adaptation to slow or rapid sequences of events. The adaptation to visual stimuli was spatially selective (in external, not retinal coordinates), pointing to a sensory rather than cognitive process. However, adaptation generalized across modalities, from auditory to visual and vice versa and from auditory to tactile and vice versa. Adaptation also generalized across formats: adapting to sequential streams of flashes affected the perceived numerosity of spatial arrays. All these results point to a perceptual system that transcends vision, audition and tactile to encode an abstract sense of number in space and in time.

Poster

Ciclo XXX

Investigation of the structural properties of MgO-based eco-sustainable cements and assessment of innovative strategies for their improvement

Monica Tonelli

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

MATERIAL SCIENCE, PHYSICAL CHEMISTRY-CHEMICAL PHYSICS

The identification of eco-compatible cement is a relevant issue in the field of building materials research. Cement formulations based on reactive periclase (MgO) constitute on the most promising emerging technologies. MgO reacts with silica sources in the presence of water, to form a gel analogue to the one present in traditional cements. In the present study, several pastes were prepared mixing MgO/silicate with Portland cement in variable ratios. The aim was to investigate in the microstructure development the effect of changing the percentage of Portland cement. The kinetics of hydration of these pastes were monitored by Differential Scanning Calorimetry, while the formation of hydrate phases were determined by Fourier Transform Infrared Spectroscopy, Differential Thermogravimetry and X-ray Diffraction. The structural properties of all samples were investigated by multinuclear Solid-State NMR. Moreover, the morphologies of the pastes has been studied by Scanning Electron Microscopy. The results show that both calcium silicate hydrate and magnesium silicate hydrate gel phase have formed. The identification of the two binders confirm the idea that it is possible to combine the ecological features of MgO-based cement with the mechanical properties of Portland cement.

Poster

Ciclo XXIX

Highly dispersed Ni catalysts over Cerium modified
mesoporous MCM-41 for hydrogen production by
ethanol steam reforming

Jorge Tovar Rodriguez

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INORGANIC CHEMISTRY, MATERIAL SCIENCE, CATALYSIS

The aim of this work is the structure modification of 1D nano structured silica to support a Ni catalyst for hydrogen production by ethanol steam reforming. Mesoporous silica MCM-41 was prepared by ultrasound assisted hydrothermal synthesis in order to achieve Cerium incorporation in the silica framework. The selected Ce/Si molar ratios for the materials were 0.02, 0.04, 0.06 and 0.08. All prepared solids exhibit hexagonal structure, high surface areas (over $546 \text{ m}^2 \text{ g}^{-1}$) and were used as catalytic support for a Nickel active phase (10% of metal loading). The catalytic activity was evaluated in the ethanol steam reforming reaction to produce hydrogen. The Ni catalyst over cerium promoted silica presented complete ethanol conversion, and hydrogen selectivity ranging from 55 to 60%. Although, production distribution is slightly dependent on Cerium content, these materials did not show catalyst deactivation after 6 h on stream and were selective towards hydrogen, carbon dioxide, carbon monoxide and methane as main products. On the other hand, bare unmodified silica as catalytic support resulted in undesired ethylene and acetaldehyde production, lower ethanol conversion (40%), less hydrogen yield (38%) and catalyst deactivation.

Poster

Ciclo XXIX

Fisher vectors over random density forests for object recognition

Francesco TurchiniDOTTORATO IN INGEGNERIA DELL'INFORMAZIONE - Informatica - Dipartimento di
Ingegneria dell'Informazione (DINFO)

COMPUTER VISION, IMAGE CLASSIFICATION

We describe a Fisher vector encoding of images over Random Density Forests. Random Density Forests (RDFs) are an unsupervised variation of Random Decision Forests for density estimation. In this work we train RDFs by splitting at each node in order to minimize the Gaussian differential entropy of each split. We use this as generative model of image patch features and derive the Fisher vector representation using the RDF as the underlying model. Our approach is computationally efficient, reducing the amount of Gaussian derivatives to compute, and allows more flexibility in the feature density modelling. We evaluate our approach on the PASCAL VOC 2007 dataset showing that our approach, that only uses linear classifiers, improves over bag of visual words and is comparable to the traditional Fisher vector encoding over Gaussian Mixture Models for density estimation.

Poster

Ciclo XXX

Climate, cities and bioenergy: development of indicators for sustainable management

Leonardo Verdi

DOTTORATO IN SCIENZE AGRARIE E AMBIENTALI - Dipartimento di Scienze
Produzioni Agroalimentari e dell'Ambiente (DISPAA)

ENVIRONMENTAL / POLLUTION, AGRICULTURE

Nowadays renewable energy sources, included biogas, are rapidly developing. However, even if biogas is widely used for heat and electricity generation, very little is known about its byproduct destination. The aim of this study is to evaluate the use of an anaerobic digestion byproduct (digestate) as a fertilizer in agriculture. The first phase of the work will be based on a field experiment to assess the response of selected agricultural crops to different kind of fertilization. In particular, mineral fertilization and different kind of digestate will be compared. Further, a specific analysis will be carried on to evaluate the environmental impacts of the different fertilization strategies. Emission rate and nutrient leaching losses will be assessed to define the sustainability of the applied cultivation techniques. The final phase of work will consist in a LCA analysis of a unit of crop product to compare the impacts of different fertilization scenarios along the entire supply chain, from fertilizer production (digestate or mineral fertilizer) to final crop harvest.

Poster

Ciclo XXX

Nuclear magnetic resonance-based metabolomics
approach to study urines of chronic inflammatory
rheumatic diseases patients

Alessia Vignoli

INTERNATIONAL DOCTORATE IN STRUCTURAL BIOLOGY - Centro di Ricerca di
Risonanze Magnetiche (CERM)

DRUGS-HEALTH, SPECTROSCOPY, METABOLOMICS

The objective of the study was to perform a metabolomic profiling of urine samples of chronic inflammatory rheumatic diseases (CIRDs) patients. The aim was to determine if the metabolic profiles of CIRDs patients varies with respect to the metabolic profiles of healthy subjects or to the ones of patients of another immun-mediated disease, i.e. multiple sclerosis (MS). Urine was collected from 39 CIRDs patients, 25 healthy subjects and 26 MS patients. Urine metabolic profiles were investigated using nuclear magnetic resonance (NMR) spectroscopy, which is most suitable for non-targeted metabolomic analysis. The ¹H NMR spectra were analyzed using PCA and PLS chemometric methodologies. Urine metabolic profiles were found to clearly discriminate between CIRDs patients and healthy controls (diagnostic accuracy 86 %) as well as between CIRDs patients and MS patients (diagnostic accuracy 83.5 %). In CIRDs patients, leucine, alanine, isobutyrate, hippurate, citrate, 3-hydroxyisovalerate, creatinine contributed to the discrimination: all of them being in a lower concentration as compared with controls or with MS patients. The metabolic profile of CIRDs patients is significantly different from both those of MS and healthy subjects. The NMR methodology applied to urines analysis is useful to obtain metabolites panels as possible markers of CIRDs.

Poster

Ciclo XXVII

Chelating agents and sensors for transition metal cations

Rania Zartit

DOTTORATO IN SCIENZE CHIMICHE - Chimica - Dipartimento di Chimica "Ugo Schiff"

ORGANIC CHEMISTRY, INORGANIC CHEMISTRY, ANALYTICAL CHEMISTRY,
SPECTROSCOPY

The objective of the research is the realization of receptors able to bind selectively and reveal the metal ions of interest environmental or biological through variations quantifiable of their fluorescence emission. We have made some chemosensors of fluorescence containing one or more polyamine units as coordination sites for metal ions and we started the study of their coordinative properties. We used as the reagents derived bis-aminal tetraaza macrocycle cyclen and as the unit fluorogenic we used quinoline and bipyridyl which in addition to their luminescent properties are also well known for their capacity to coordinate metal ions. They were synthesized and characterized three new ligands L1 containing a unit of polyamine cyclen with hung two units of quinoline and two acetate groups and L2 constituted from two units of cyclen connected by unit dipyritydyl while L3 formed from two units of cyclen connected by two units of dipyritydyl. The analysis of coordinative properties of L1 L2 against metal ions showed that they are a potential sensor for Zn that its the only ion able to increase while other ions dont increase or reduce the intensity through potentiometric measurements absorption spectroscopy UV-vis and fluorescence emission spectroscopy. L3 still under study.

NOTE

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NOTE

Credits

Organization Committee: Lorenzo Cortese, Dario Di Fina, Giulia Dotta, Eleonora Mercatelli, Riccardo Muzzioli, Barbara Olmi, Erica Parisi, Lorenzo Pattelli, Sofia Pazzagli, Federica Scaletti, Erica Secci, Leonardo Verdi.

Chair (rigorosamente in ordine sparso): Francesco Carlà, Pasquale Totaro, Lorenzo Poggini, Enrico Ravera, Giuseppe Cucinotta, Fabrizio Sgrignuoli, Pietro Lombardi, Niccolò Caselli, Eduardo Grossi, Enrico Luchinat, Francesco Fidolini, Giovanna Poggi, Claudia Crocini, Eros Quarta.

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Polo Scientifico, Sesto Fiorentino (FI)