



Università degli Studi di Trieste



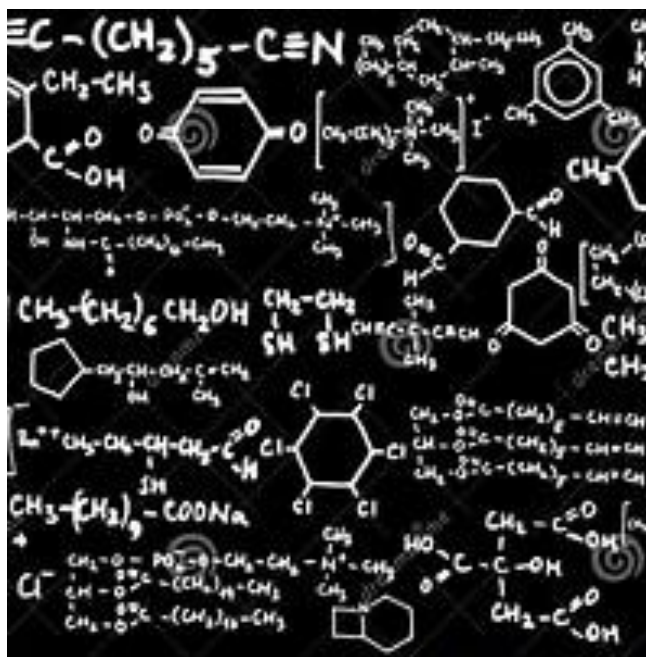
**UNIVERSITÀ
DEGLI STUDI
DI UDINE**

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Università degli Studi di Udine

CONVEGNO SCIENTIFICO

I giovani e la Chimica in Friuli Venezia Giulia



UDINE, 9 Novembre 2018

Aula Auditorium – DI4A
Via del Cotonificio 108

Il Consiglio Direttivo della Sezione Friuli Venezia Giulia della Società Chimica Italiana, rinnovando un evento culturale già sperimentato con successo negli scorsi anni, ripropone l'incontro scientifico tra le realtà universitarie regionali organizzando il convegno "I Giovani e la Chimica in Friuli Venezia Giulia". Tale occasione di incontro tra i giovani non-strutturati offre loro l'opportunità di presentare i risultati del proprio lavoro di ricerca più recente. Lo scopo principale è di promuovere la conoscenza e l'integrazione dei gruppi di ricerca universitari regionali proiettando un'immagine giovane e vitale della Chimica all'esterno del mondo accademico. Nel programma è inserita la conferenza plenaria del Prof. Marco Bandini focalizzata sulla funzionalizzazione di composti arenici. Al termine dei lavori seguirà l'assemblea annuale della sezione Friuli Venezia Giulia.

Programma

Ore 9.00 – 9.15 *Saluti ed apertura lavori*

*Chairperson: **Lanfranco Conte***

Ore 9.15 **OC1- Anna Lenarda** Università di Trieste

Title: "Selective H₂O₂ electrocatalytic generation by cobalt@N-doped graphitic carbon core-shell nanohybrids"

Electrocatalytic oxygen reduction (ORR) is emerging as an interesting synthetic strategy to produce hydrogen peroxide (H₂O₂) in a green and sustainable way. N-doped graphitic carbon embedding cobalt nanoparticles prepared from imidazole precursor is proposed as an advanced material able to selectively trigger the ORR to form H₂O₂. The Faraday Efficiency calculated is almost 100% at very positive applied potentials and the production of H₂O₂ proceeds with high rates (49 mmol g⁻¹ h⁻¹) and good current densities (about -0.8 mA cm⁻² at 0.5 V vs RHE). The dependence of its totally selective behavior has been studied and ascribed to different concomitant features, such as the textural properties, the nature of the metal, the N-type distribution, the acidic environment and the applied potential.

Ore 9.30 **OC2- Maila Danielis** Università di Udine

Title: Outstanding methane oxidation performance over innovative Pd-embedded ceria catalysts prepared by dry methods

The upcoming stricter legislation on CH₄ emissions at tailpipe has pushed towards the development of more efficient methane oxidation catalysts. Pd/CeO₂ catalysts are especially active and their performance is closely related to the nanoscale Pd-Ce interaction. With the aim of promoting it, a novel dry milling procedure was developed resulting in materials with outstanding activity and improved stability. These catalysts exhibit a unique morphological structure where Pd is embedded in an amorphous ceria layer covering the ceria crystallites. The enhanced catalytic properties were correlated with the peculiar Pd-O-Ce interface created at nanoscale by mechano-chemical interactions induced by the milling process.

Ore 9.45 **OC3- Irene Marcovich** Università di Trieste

Title: "Structural studies on enzymes: a bacterial polymerase and a human kinase"

The Wzx/Wzy dependent pathway is an essential step for the LipoPolySaccharide correct assembly. This polymer plays a key role in bacterial survival. Due to the important roles played by Wzx to this pathway and

its species specificity, Wzx structure determination would help the design of antibiotics able to treat superbug infections.

GSK3 β is a kinase involved, together to CK1 δ , in the hyperphosphorylation of protein Tau, one of the pathological hallmarks of Alzheimer's Disease. The determination of the X-ray structure of GSK3 β in complex with SR90, a dual GSK3 β -CK1 δ inhibitor, revealed its covalent bond to GSK3 β confirming computational modeling simulations.

Ore 10.00

OC4- Caterina Deganutti

Università di Trieste

Title: The P-Type ATPase Neo1: Structural insights into yeast flippases

The P-IV ATPases, eukaryotic membrane proteins (flippases), are related in human to cholestatic disease, Alzheimer's disease, obesity and type 2 diabetes.

The yeast *Saccharomyces cerevisiae* expresses 5 different P-IV ATPases, among them the most interesting one is Neo1. With the final aim to elucidate structural details of Neo1, we set up an overexpression protocol in different conditions (temperature, metals or DMSO addition). For the detection and quantification of Neo1 by UV excitation, the protein was fused with GFP. We are testing now different chromatographic methods and detergents to stabilize the protein and crystallize it for X-ray diffraction.

Ore 10.15

OC5- Elena Pavoni

Università di Trieste

Title: Estuarine trace elements distribution: phase partitioning and role of salinity gradient in the river mouths of the Gulf of Trieste

Potentially harmful elements (PHEs) are supplied to estuarine environments by freshwater inputs affected by anthropogenic sources. This work aims at the evaluation of PHEs (Pb, Hg, Cs, As, Zn, Cu, Ni, Co, Fe, Mn) partitioning among suspended particulate matter, retentate and permeate fractions in the river mouths of the Gulf of Trieste (Isonzo, Timavo and Dragonja rivers).

Significative concentrations of PHEs were detected in the particulate and dissolved fractions and to a certain extent PHEs were associated to the retentate fraction. PHEs showed a non-conservative behavior and salinity gradient appear to have an important role in their mobility and partitioning.

Ore 10.30

OC6- Chiara Conchione

Università di Udine

Title: Migration of hydrocarbon contaminants from packaging into food: a case of study

Packaging as well as other food contact materials (FCM) such as adhesives and printing inks, are the main sources of chemicals in food products and beverages. The aim of this study was to conduct a survey about boxes used for pizza transport in particular regarding two kind of contaminants: mineral oil hydrocarbons (MOHs) and polycyclic aromatic hydrocarbons (PAHs). These substances are quantified in different samples of pizza boxes that were taken directly in pizza restaurants in the North-East and South Italy, contamination sources are investigated. Finally, migration test is carried out using simulant Tenax® in order to evaluate their potential migration.

Ore 10.45 – 11.15 *coffee break*

Ore 11.15

OC7- Elisa Bernes

Università di Trieste

Title: Core-electron excitations in thiophene derivatives as building blocks of nanostructured materials: a computational DFT/TDDFT study

The electronic structure of a promising class of building blocks in organic molecular electronics (thiophene-T, benzo[*b*]thiophene-BBT and dibenzothiophene-DBT) in the gas phase has been investigated by combining the outcomes of Near-Edge X-ray-Absorption Fine-Structure (NEXAFS) and X-ray Photoemission Spectroscopy (XPS) at the C K-edge and the S L_{II,III}-edges with those of density functional theory (DFT) and of Time-Dependent DFT calculations. The C1s NEXAFS and S2p spectra are informative of both low-lying delocalized π^* and higher-lying localized $\sigma^*(\text{C-S})$ states. The evolution of the C1s NEXAFS and XP spectra suggests a stabilizing effect due to increased aromaticity (more pronounced from T to BBT), while the nature and the energy position of the most intense S2p NEXAFS spectral features is conserved, revealing a much lower dependence on the degree of annulation.

Ore 11.30

OC8- Matteo Busato

Università di Udine

Title: Structural and Thermodynamic Features of the Zn(II) ion in Room Temperature Ionic Liquids

Thanks to some unique properties, room temperature ionic liquids (RTILs) have been proposed as a "green" alternative to organic solvents in extraction processes of transition and rare-earth metals from aqueous solutions.

In this work, the solvation of Zn(II) has been studied in the [C_nmim][Tf₂N] (n=1,2: 1-ethyl-3-methylimidazolium and 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide) RTILs both in dry and wet conditions by means of molecular dynamics simulations (MD) and X-ray absorption spectroscopy (XAS). The results allowed to obtain structural and thermodynamic parameters of fundamental importance to describe metal ions solvation in these solvents and will help to improve new application involving metals and RTILs.

Ore 11.45

OC9- Rosario Figliolia

Università di Udine

Title: Novel Ruthenium Carboxylate Complexes Synthesis and Catalytic Applications

Starting from Ru(OAc)₂(PPh₃)₂, well-defined novel diacetate ruthenium complexes bearing the electron-rich diphosphines of the type Ru(OAc)₂(CO)_n(PP) (with n= 0, 1 and PP = DiPPF, DCyPF) have been synthesized in very good yields. Those complexes showed high reactivity in hydrogenation, transfer hydrogenation and *N*-alkylation reactions. The Ru(OAc)₂(CO)(DⁱPPF) in particular, attained high reactivity and productivity (TOF and TON up to 10³ and 10⁵, respectively) in the reduction of neat untreated α,β -unsaturated aldehydes in solvent less conditions without a base.

Ore 12.00

OC10- Marina Kurbasic

Università di Trieste

Title: Self-Assembling Peptides into Antimicrobial Hydrogels

Antimicrobial peptides are an interesting class of therapeutics. It was recently reported that the tripeptide ^DLeu-^LPhe-^LPhe displays mild antimicrobial activity when it forms a supramolecular hydrogel at physiological conditions, yielding a soft material that does not display cytotoxicity or hemolytic activity *in vitro*. Based on

this sequence, a series of short peptides has been prepared to understand the structure-activity relationship. Importantly, the antimicrobial activity is only observed in the hydrogel state, indicating a key role played by the supramolecular structures. This offers the possibility to control antimicrobial activity, simply by the assembly or disassembly of the superstructures *on demand*.

Ore 12.15

OC11- Maria Cristina Cringoli

Università di Trieste

Title: Functional materials based on nanocarbons

Incorporation of carbon nanomaterials in short peptide hydrogels is a useful means to design new composite biomaterials with acquired properties. The self-assembly of a tripeptide containing both D- and L- amino acids at specific positions is evaluated in presence of four different nanocarbons (carbon nanodots, carbon nanotubes, graphene oxide and carbon nanohorns) to study the effect of their shape and dimension. Supramolecular hydrogels at physiological conditions are obtained in all cases. Viscoelastic properties are affected by the presence of the nanocarbons and a self-healing ability was observed only upon inclusion of carbon nanotubes in the system.

Ore 12.30

OC12- Jacopo Segato

Università di Udine

Title: Homogeneous Gold(I) catalysis for hydration of alkynes in solvent and acid-free environment

Engineering the reaction to reduce or eliminate the use or generation of hazardous substances in according to the twelve principles of the green chemistry, has become a must nowadays. In this contribution, L-Au-X [L= 1,3-bis(2,6-di-isopropylphenyl)-imidazol-2-ylidene {NHC^{IPr}}, tris(3,5-bis(trifluoromethyl)phenyl)phosphine {PArF}, bis(imino)acenaphthene-1,3-bis(2,6-di-isopropylphenyl)dihydroimidazol-2-ylidene {BIAN}, bis(*tert*-butylamino)methylidene {NAC}, 2-(di-*tert*-butylphosphino)biphenyl {JohnPhos}, PCy₃, PPh₃, tris(2,4-di-*tert*-butylphenyl)phosphite {POR₃}, X⁻ = Cl⁻, OTf⁻, OTs⁻] were tested as catalysts for the hydration of alkynes in neat and acid-free conditions, using tetra-butylammonium trifluoromethanesulfonate as phase-transfer. A complete rationalization of the ligand and counterion effects enabled us to develop a highly efficient methodology even for the hydration of inactive diphenylacetylene performing the catalysis in acid- and silver-free conditions with: low catalyst loading (0.01% with respect to the substrate), high TON (3400) and TOF (435 h⁻¹) at 120 °C, low E-factor (0.03), and high EMY (77).

Ore 12.45

OC13- Rudy Calligaro

Università di Trieste

Title: Polypyridyl Ru(II) complexes: new synthetic approaches towards bis-heteroleptic derivatives from *cis*-locked precursors

Ru(II)-polypyridyl complexes, by virtue of their unique photophysical and redox properties, find applications in a wide range of fields. For this reason the development of efficient synthetic procedures for bis- and tris-heteroleptic compounds is of particular interest. The well-known *cis*-[RuCl₂(dmsO)₄] complex could be a useful precursor, was found to be rather unselective when reacted with polypyridyl ligands (chel). With the purpose of avoiding this problem, *cis*-locked precursors such as [K][*fac*-RuCl(dmsO)₃(η²-mal)] (mal = malonate) were synthesized and their reactivity with the model diimine ligands was investigated. Disubstituted [Ru(chel)₂(η²-mal)] derivatives were obtained in rather good yields. The malonate ligand was easily and selectively replaced under acidic conditions by a second diimine ligand (chel'), affording the bis-heteroleptic complexes [Ru(chel)₂(chel')][PF₆]₂ in excellent yields.

Ore 13.00

OC14- Cristian Rosso

Università di Trieste

Title: Atom-Transfer Radical Additions Triggered by the Photochemical Activity of Perylene Diimides (PDIs)

Visible-light photocatalysis has recently emerged as a powerful strategy for radical chemical transformations. In 2014, prof. König exploited the ability of perylene diimides (PDIs) to function as photocatalysts for the reduction of aryl halides. Despite the excellent opto-electronic properties of PDIs, their application in photochemistry remains rare. We employed a PDI as effective photocatalysts for an Atom-Transfer Radical Addition reaction between terminal olefins and perfluoroalkyl iodides under blue-light irradiation. A very low amount of PDI leads to the formation of the iodo-perfluoroalkyl compounds in high yields. These can be used as building blocks to prepare new relevant chemical species

Pausa pranzo

*Chairperson: **Daniele Zuccaccia***

Ore 15.00

Plenary lecture- Marco Bandini

Università di Bologna

Title: New catalytic “decorative” protocols of arenes

Ore 15.50 – 16.00 *Chiusura dei lavori*

Ore 16.00

Assemblea Sezione SCI Friuli Venezia Giulia

La Presidenza e il Consiglio Direttivo della Sezione FVG della SCI ringraziano quanti hanno contribuito alla realizzazione del Convegno ed in particolare il Dipartimento di Scienze agroalimentari, ambientali e animali dell'Università di Udine