

O Colóquio do Departamento de Química Fundamental acontece todas as quarta-feiras às 16:00 hs no Auditório Prof. Benício de Barros Neto. Durante o semestre de 2015.2, contactar o Prof. Roberto Lins para agendamento e divulgação de apresentações.

Colóquio Especial - 02 de novembro as 10h00 - Prof. Carlos Albero Montanari, IQ, USP-SC

**Energética e Caracterização Estrutural da Cisteína Protease Vruzaína Usando Biocalorimetria e Cristalografia de Raios X**

Colóquio Especial - Segunda-feira 30 de novembro das 10h00 as 12h00, 14h as 15h e 15h as 16h 30 de Novembro.

De 10h as 12h - Prof. Julien Gautrot, School of Engineering and Material Sciences, Queen Mary University of London, UK

**Polymeric Biocompatible Materials.** This lecture will cover the chemical synthesis, physical-chemical characterization and applications of polymer brushes as biocompatible surfaces. These topics will be explored at an introductory level for graduate students in the chemical, materials and life sciences. The content of this lecture will serve as basis for the afternoon presentations on the synthesis of peptide based biomaterials via thiol-ene chemistry

and the application of polymer brushes for gene delivery.

**30 de Novembro. De 14h as 15h - Dr. Danyang Li, School of Engineering and Material Sciences, Queen Mary University of London, UK**

**Study of DNA-PDMAEMA Brush Interactions for Application to Gene Delivery.** Gene therapy has shown promise in therapies for various genetic diseases and cancers, a gene carrier or vector is needed to escort negatively charged nucleic acids through cell membranes. Poly(2-dimethylaminoethyl methacrylate) (PDMAEMA) brushes obtained via ATRP have emerged as an attractive technique offering precise control over macromolecular structure, order, and functionality to design multifunctional materials for a variety of applications in bioengineering, especially in gene delivery. This project is mainly based on investigating the PDMAEMA brush behaviour under different conditions and brush-DNA interactions to better understand the gene delivery process. PDMAEMA brushes with different length and density were prepared both on flat surfaces (e.g. silicon wafer and gold surface) and 310 nm silica nanoparticles. The initial study was focused on brush behaviours (e.g. swelling and collapse) of those PDMAEMA coated substrates as well as PDMAEMA brush decorated silica nanoparticles on different stimuli-responsive (e.g. salt, pH) with ellipsometry and zetasizer. Followed by deeper understand of brush-DNA interactions by surface plasmon resonance (SPR), it displays that DNA-brush association and disassociation process were effected not only by the brush coated surface properties, but also by the length and shape of DNA. Finally, PDMAEMA brush decorated silica nanoparticles were used as potential non-viral vectors for in vitro gene delivery with HaCaT cells. As in consideration of application to living system, the effect on transfection efficiency of some commonly used salt in biomedical areas, such as PBS, NaCl, HEPES were investigated.

**30 de Novembro. De 15h as 16h - Burcu Colak, Graduate Student, School of Engineering and Material Sciences, Queen Mary University of London, UK**

**Peptide based biomaterials via thiol-ene chemistry.** Photo initiated thiol-ene chemistry was

generated as a tool to produce a series of biomaterials. We characterised the thiol-ene coupling efficiency under biologically relevant conditions with a range of thiols and alkenes, using NMR spectroscopy and HPLC. Understanding the chemistry enabled to establish the parameters required to use this tool for the production of bioactive hydrogels and biofunctional surfaces. A series of polymers were linked with biofunctional crosslinkers to generate bioactive hydrogels of varying chemical and mechanical properties. Since amino acid cysteine contains a thiol group, a series of peptides with various features could behave as crosslinkers or tethers to create biofunctionality in the hydrogel. Thiol-ene was used to introduce selected biofunctions into the hydrogel, integrin binding sequences for adhesion and enzyme cleavable sequences for degradable hydrogels. Some polymeric brushes have anti-fouling properties; this makes these surfaces a good tool for the study of material-cell interfaces. Integrin binding peptides were chemically bonded to these surfaces and their cell responses were measured. Thiol-ene was also used as a tool for photo-patterning onto these surfaces.

26 de Outubro - Dr. Yi-Chieh, **University of Strathclyde, Scotland**

**Innovative Multipurpose NIR Spectroscopy for Real-Time Physical and Chemical Characteristics of Dense Media** Optical measurements can be a relatively simple and effective way to identify the differences in the products since the differences in the chemical and physical characteristics of pharmaceutical products will manifest as differences in their optical (scattering and absorption) properties. We investigate the optical properties of dense media using innovative spatially and angularly resolved diffuse reflectance (SARDR) measurements in visible-near infrared (vis-NIR) wavelength region. The scattering and absorption optical properties are analysed using physical-based models which resolve complex light propagation behaviour in turbid and dense media. Several types of systems which are applied to evaluate the performance of the methodology will be presented.

14 de Outubro - Dr. Remo Simonetti, **University of Genoa, Italy**

**Hyperspectral image analysis and chemometrics: chemical information pixel by pixel**

Nowadays, image analysis is becoming more and more important because of its ability to perform fast, low-cost and non-invasive investigations. The denomination “image analysis” encloses studies on classical grey scale or RGB images, analysis of images collected using few spectral channels and, more recently, the so-called hyperspectral images, in which a considerable number of channels – typically hundreds or thousands – constitute the spectral dimension. A wide number of analytical techniques – ranging from ultraviolet, visible and infrared (near, mid and far) to Raman spectroscopy, and even to X-ray fluorescence, mass spectrometry, and nuclear magnetic resonance – can be exploited to supply hyperspectral images, for very efficient chemical and positional characterisations. In fact, hyperspectral images are usually structured as three-dimensional data arrays constituted by two spatial dimensions and one spectral dimension. In the recent decades, the chemometric community joined this field firstly introducing existing tools (namely, exploratory analysis, classification and regression techniques) appropriately modified to fit the particular characteristics of image structures, and later by developing tools specifically targeted for these peculiar 3D data arrays. In the present talk, the principal chemometric strategies for managing hyperspectral data will be described and critically discussed. An exemplificative case study of FT-Raman HSI (Hyper Spectral Imaging) and multivariate data treatment will be presented, concerning chemical characterisation of individual particles from atmospheric aerosols at the micrometre scale. Confocal Raman micro- spectrometry – which combines the spatial resolution of optical microscopy and the molecular analysis capabilities of Raman scattering – allowed to acquire molecular information from individual micrometre-sized aerosol particles: a key task to assess their impacts on human health and climate changes.

**23 de Setembro - Prof. Andrea Perali, University of Camerino, Italy.**

**High temperature electron-hole superfluidity in double bilayer graphene**

12 de Agosto - Prof. **José Manuel Amigo, University of Copenhagen, Denmark**

**One analytical chemist between food scientist. Why? - Multivariate Perspective of complex data analysis**

Short CV: José Manuel Amigo (born 1978) obtained his Ph.D. (Cum Laude) in Chemistry from the Autonomous University of Barcelona, Spain. Since 2007 he has been employed at the

Department of Food Science, Spectroscopy and Chemometrics group of the University of Copenhagen, Denmark as associated professor. Current research interests include hyperspectral analysis, process analytical technologies and Chemometrics. He has authored more than 70 publications (57 peer-reviewed papers, books, book chapters, proceedings, etc.) and given more than 40 conferences in international meetings. José has supervised or is currently supervising 7 masters, post docs and Ph.D. students and he is an editorial board member of four scientific journals within chemometrics, pharmaceutical sciences and analytical chemistry. He has recently received the “2014 Chemometrics and Intelligent Laboratory Systems Award”.

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08 de Julho - Prof. Boaventura Freire dos Reis, **Centro de Energia Nuclear na Agricultura, USP**

**Análise em Fluxo: Da Seringa à Multicomutação**

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08 de Abril - **Ernesto Jimenez Villar, dQF, UFPE**

**Localization transition and random lasing in a colloidal suspension composed of core-shell nanoparticles (TiO<sub>2</sub>@Silica)**

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01 de Abril - Prof. Petrus Santa Cruz, **dQF, UFPE**

## Perspectivas e Implicações Acadêmicas da Pós-Estatuinte

## Colóquios Apresentados Anteriormente

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