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SEMINAR

Thursday, 15th January, 12.00 pm, Seminar Room

Host: Prof. Luis Liz-Marzán

Plasmonic Nanostructures: Identification, detection and killing of *Escherichia Coli*

Sabine Szunerits
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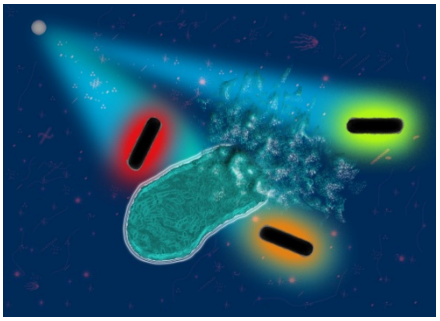
Like any other pathogen, *Escherichia coli* (*E. coli*) shows a high reproductive rate under optimal conditions posing a major threat to human health and society at large. The development of bacterial strains that are multiresistant to antibiotic treatments has currently reached a critical level, invalidating major antimicrobial drugs for clinical use. These and other considerations have seen an increased interest in the development of non-biocidal anti-infective strategies as alternatives to antibiotics, as these would be expected to show reduced tendency to potentiate resistant strains evolving.



We have recently shown that an appealing strategy is the use of anti-adhesive molecules that target specifically initial interaction events between bacteria and surfaces, steps critical for effective colonization and establishment of biofilm by pathogens.[1] Motivated by this work, we developed plasmonic interfaces which allowed to investigate in an easy and efficient manner the adhesion behavior of different *Escherichia coli* strains as well as its selective analytical detection.[2] We took furthermore advantage of the excellent light absorption properties of graphene-coated gold nanorods in the near-infrared (NIR) to photothermally kill selective gram-negative pathogens up to 99% in 10 min.[3]

References :

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SEMINAR

Wednesday, 28th January, 12.00 pm, Seminar Room

Host: Dr. Luca Salassa

Benefits from Electronic Structure Computing. A Case Study: Modeling of Electron Transfer triggered by Quantum Dot Photoactivation.

Ivan Infante[a], Jon M. Azpiroz[a], Nina Gómez Blanco[b], Emmanual Ruggeiro[b], Jesus M. Ugalde[a], Juan C. Mareque-Rivas[b], Luca Salassa[b,c]

[a] Kimika Fakultatea, Euskal Herriko Unibertsitatea and Donostia International Physics Center, P. K. 1072, 20080 Donostia, Euskadi, Spain.

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The lecture will first briefly describe the research programme being pursued by the Quantum Chemistry Group at Donostia and then will concentrate on the title subject as a way to illustrate the benefits that can be expected from close scientific collaborations with theoreticians.

Semiconductor Quantum Dots (QD) have recently raised a lot of interest as lightinduced electron transfer (ET) activators, with very promising results in varios research areas like photoactivatable protein inhibitors, photodynamic therapy (PDT), and photocatalysis.

In this lecture we discuss the results from a combination of Density Funtional Theory (DFT) and timedependentDFT (TDDFT) calculations and a number selected experiments in the context of rationalizing the ET process from a core–shell CdSe@ZnS QD into a Pt(IV) anticancer agent, namely, cis,cis,trans-$[Pt^{IV}(NH_3)_2(Cl)_2(O_2CCH_2CH_2CO_2H)_2]$ (**1**).

Pt(IV) complexes have been extensively studied as prodrugs whose activity can be switched on in vitro and in vivo by biological reductants or by light excitation. Quantum Dot mediated photoactivation of anticancer complexes is now becoming a promising technique for its implementation in vivo trails, and, in this lecture, will show one example of a fruitful cooperation between theory and experiment in order to unveil the prodrug's photoactivation mechanism.

We found that direct adsorption of the complex on the QD surface results in large electronic coupling between the LUMO (lowest unoccupied molecular orbital) of the excited QD* and the LUMO+1 of **1**, providing the driving force to the lightinduced release of the succinate ligands from the Pt prodrug. As confirmed by photolysis experiments performed a posteriori, DFT highlights that QD photoactivation of **1** can favor the preferred formation of Pt(II) photoproducts, providing valueable hints for the design of novel hybrid Pt(IV)-semiconductor systems where the photochemical activation processes can be tuned.

References :

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I. Infante, J. M. Azpiroz, N. Gomez Blanco, E. Ruggiero, J. M. Ugalde, J. C. Mareque-Rivas, L. Salassa, *"Quantum Dot Photoactivation of Pt(IV) Anticancer Agents: Evidence of an Electron Transfer Mechanism Driven by Electronic Coupling*", The Journal of Physical Chemistry C, vol.118, iss.16, pp 8712–8721 (2014).

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SEMINAR

Wednesday, 4th March, 12.00 pm, Seminar Room
Host: Prof. Luis Liz-Marzán

Colouring Atoms in Three Dimensions

Sara Bals
Department of Physics
University of Antwerp, Belgium

Nanosystems that are being investigated within the field of physics, biology and chemistry are becoming smaller and more complex. As a consequence, higher demands are being put to microscopic and nanoscopic characterization techniques as well. New developments within the field of transmission electron microscopy (TEM) allow investigating these systems at the atomic scale, not only structural, but also from chemical and electronic point of view. However, one should never forget that all these techniques only provide a two-dimensional (2D) projection of a three-dimensional (3D) object. To overcome this problem, electron tomography has been used in an increasing number of studies over the last decennium. Nevertheless, it is still not straightforward to push the resolution below the nanoscale in 3D. This relies on the combination of state-of-the-art electron microscopes and advanced computational procedures to transform the 2D images into a 3D reconstruction.

One of the possibilities to perform electron tomography with atomic resolution is by applying reconstruction algorithms based on compressive sensing. We hereby exploit the fact that nanomaterials at the atomic scale are sparse. The methodology was applied for Au nanorods and the crystal lattice of the nanorods could be reproduced without using prior knowledge on the atomic structure! From these reconstructions, the boundary facets of different rods have been precisely determined and the reconstruction can serve as a starting point to investigate strain in 3D [1]. More recently the technique was applied to visualize crystal defects at the atomic scale and to distinguish between different types of atoms [2]. These investigations will yield more insight on the connection between properties and structure of a broad range of nanostructures.

An alternative approach to resolve the chemical composition of complex nanostructures in 3D is by using energy dispersive X-ray (EDX) mapping. Early 3D EDX experiments were complicated by the specimen-detector geometry, but recent efforts enable 3D EDX in an optimized manner. 3D EDX reconstructions were used to understand the morphological and chemical transformations during a Galvanic replacement process [3]. Finally, the ability to map valence in 3D will be demonstrated [4].

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SEMINAR

Friday, 6th March, 12.00 pm, Seminar Room
Host: Prof. Luis Liz-Marzán

Magnetic nanoparticles: A precision tool for cell imaging and activations

Jinwoo Cheon
Department of Chemistry, Yonsei University, Korea
jcheon@yonsei.ac.kr

One of the important trends of next-generation biomedical sciences is the development of new tools that can accurately image, identify, and execute desired missions in a selectively programed manner. Nanotechnology is among one of the essential platform tools for targeted imaging, therapy, and simultaneous monitoring of therapeutic efficacy. In this talk, I will discuss magnetic nanoparticles as a core platform material and tool for a variety of functionalities such as sensing, targeting and signaling of cells in a selective and efficient way. Their unique utilizations in highly accurate dual-modal MR imaging, therapeutic hyperthermia of cancer cells, controlled drug/gene delivery, and molecular level cell signaling and cell fate control will be discussed.

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SEMINAR

Monday, 16th March, 12.00 pm, Seminar Room
Host: Prof. Luis Liz-Marzán

Recent Topics in Nanotechnology: Gold Atom (Crown Jewel) Catalysts and Hybrid Organic Thermoelectric Films

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Nanoscience and nanotechnology are now applied to various fields in the world. Here I will present two topics developed in our group quite recently.

The first topics is concerned with single-atom catalysts of so-called Crown Jewel catalyst which have a top gold atoms on palladium clusters and highly active for aerobic oxidation of glucose (*Nature Materials*, **2012**). Here, we prepared Crown Jewel-structured (Ir/Pd)/Au trimetallic nanoclusters having the highest catalytic activity for the glucose oxidation by galvanic replacement reaction of Ir/Pd bimetallic nanoclusters with Au atoms at top positions. The high activity of the top Au atoms can be explained by the electronic properties of top Au atoms (*Advanced Materials*, on-line pub., **2015**).

The second topic is concerned with conversion of waste heat energy to electric energy with flexible organic thermoelectric devices, which have much advantages compared with traditional inorganic ones. The hybrid organic thermoelectric materials prepared by using nanoparticles of a polymer complex, carbon nanotubes and poly(vinyl chloride) have been discovered to be developed without conducting polymers like PEDOT-PSS and have a high thermoelectric performance (ZT = 0.3). The hybrid materials are stable and easily applied to constructing flexible thermoelectric devices with high maximum electric power (*Advanced Materials*, accepted for publication, **2015**).

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SEMINAR

Monday, 13th April, 12.00 pm, Seminar Room

Host: Prof. Luis Liz-Marzán

Protein-based functional nanostructures and multifunctional nanoparticles

Aitziber L. Cortajarena[1,2]

[1] IMDEA Nanoscience, c/ Faraday, 9, Ciudad Universitaria de Cantoblanco 28049, Madrid (Spain);

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Protein-based functional nanostructures

The precise synthesis of nano-devices with tailored complex structures and properties is a requisite for their use in nanotechnology and medicine. Bottom-up self-assembly that relies on highly specific biomolecular interactions of simple components, is an attractive approach for nanostructure templating.

Here, we use self-assembling protein building blocks as templates for nanofabrication. In nature, protein assemblies govern sophisticated structures and functions, which are inspiration to engineer novel assemblies by exploiting the same set of tools to create nanostructures with numerous potential applications.

We present the design of a collection of protein-based functional nanostructures and materials using modular repeat proteins as building blocks, in particular designed consensus tetratricopeptide repeats (CTPRs) which stability and function and self-assembly properties can be tuned.

Multifunctional nanoparticles

Nanomedicine nowadays offers novel solutions in cancer therapy and diagnosis by introducing multimodal treatments and imaging tools in one single formulation. Nanoparticles acting as nanocarriers change the solubility, biodistribution and efficiency of therapeutic molecules reducing their side effects. In order to apply successfully these novel therapeutic approaches, efforts are focused on the biological functionalization of the nanoparticles to improve the selectivity toward cancer cells. Here, we show the use of multifunctional magnetic nanoparticles (MNP) for selective drug delivery to cancer cells. Firstly, we demonstrate the targeting of MNP functionalized to different cancer cell lines, and verify the specificity. In addition, we show the drug delivery potential of the MNP by the killing of cancer cells using multifunctional MNP with both targeting moieties and chemotherapy drugs.

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SEMINAR

Thursday, 16th April, 12.00 pm, Seminar Room
Host: Prof. Luis Liz-Marzán

Attractive iron oxide nanoparticles for clinical applications

Anna Roig
Senior Researcher and Deputy Director ICMAB-CSIC
Nanoparticles and Nanocomposites Group (www.icmab.es/nn)

Iron oxide nanoparticles are becoming an important class of materials in nanomedicine since they can be used in MRI as contrast agents as well as for therapeutical purposes. The talk will include a brief introduction to iron oxide nanoparticles and the characteristics that make them attractive in the health sector. Some synthetic approaches used in the group will be described including the fabrication of gold-iron oxide nanocrystals. A collaborative project with the Vall d'Hebron Hospital using magnetic nanoparticles and nanocapsules to promote angiogenesis as a brain neurorepair therapy after stroke will be also presented.[1] [2] [3]

[1] Rapid synthesis of water-dispersable SPIONs by microwave assisted route for safe labeling of endothelial progenitor cells, Carenza et al. *Acta-Biomaterialia 10 (2014) 3775 DOI:10.1016/j.actbio.2014.04.01*

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Friday, 17th April, 12.00 pm, Seminar Room
Host: Prof. Luis Liz-Marzán

Directed Self-Assembly of Janus Nanoparticles for SERS Applications

Denis Rodríguez Fernández
BioNanoPlasmonics Lab

The work presented in this thesis focuses on the preparation of new types of Janus nanoparticles made of gold and silica. This type of particles exhibit different properties at opposite sides, opening the way to prepare new materials with combined properties and showing potential applications in self-assembly, catalysis or detection. [1]

A wide variety of synthetic approaches have been developed to control the size, geometry and the optical properties of the Janus particles. [2-5] Morphological changes have been deeply characterized by electron microscopy and were correlated to modifications in their optical properties. In addition, computer simulations of the optical properties were carried out in order to compare experiments with theory.

The directed self-assembly of these particles is also presented, showing potential applications as surface enhanced Raman scattering (SERS) reporters. [5]

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[5] D. Rodríguez-Fernández, J. Langer, M. Henriksen-Lacey, L. M. Liz-Marzán, *Chem. Mater.* **2015**, accepted.

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SEMINAR

Wednesday, 27th May, 12.00 pm, Seminar Room

Host: Dr. Niels C. Reichardt

The Significance Of Glycosylation To The Biopharmaceutical Industry

Dr. Richard Easton
Services Team Leader, Carbohydrate Analysis
SGS Life Sciences, UK

Glycosylation is an abundant post-translational modification present on glycoproteins from a wide variety of biotechnologically important cell lines. The glycosylation of these different glycoproteins can have a significant impact on the efficacy of the drug and thus the structural nature of the glycans must be understood in order to be controlled. Furthermore, regulatory authorities require a complete structural knowledge of biotherapeutics and thus glycosylation must be fully characterised in order to also meet this requirement. Analytical techniques exist that allow extremely detailed investigative analysis of diverse glycan structures found on glycoproteins produced in different cell systems. Detailed structural analysis is also important in production of biosimilars, where methods need to be able to highlight similarities and differences between the glycosylation profiles of different samples. The nature and significance of glycosylation as well as how analytical methods can be applied to solve the glycan structures in these complex systems will be discussed.

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SEMINAR

Friday, 29th May, 11.00 pm, Seminar Room

Host: Prof. Luis Liz-Marzán

Sophisticated nanopatterned metal networks for transparent flexible electrodes and optoelectronic applications

Michael Giersig
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Helmholtz Zentrum Berlin, Institute of Nano-architectures for Energy Conversion, Hahn-Meitner-Plattz 1, 14109 Berlin, Germany

Novel high performance applications in optoelectronics require highly transparent and highly conductive electrodes (TCEs) for high yields, which are ideally applicable to flexible surfaces. At present, transparent conductive oxides such as indium tin oxide are the dominant TCE materials used in these technologies. Due to the decreasing supply of raw materials, namely indium, at odds with the increasing usage of the above technologies, new alternative TCE materials such as metal networks are under investigation.

In this presentation we demonstrate regular[1] and irregular[2,3] metal networks fabricated employing standard lithographic and metal nanoparticle self-assembly methods[3,4] where the transparency and sheet resistance can be tuned by simply changing the geometrical dimensions of the metal network.[1] To this end, nanosphere lithography is discussed as a promising and inexpensive technique which builds the foundations for several metal network geometries ranging from periodically perforated metal films over metal grating to irregular networks.
Herein, we show results from transparent silver networks.[1-3] Optical, structural and electronic properties of these networks are investigated using optical, four-point probe and SEM measurements. Sheet resistances as low as 3 Ohm/Sq and an average optical transmission greater than 70% were achieved. A simple geometric model for predicts percent transmission values up to 90% promising competitiveness with transparent conductive oxides. Finally, we demonstrate the applicability of these networks to flexible surfaces for their potential use as transparent and flexible metal electrodes in optoelectronic applications.

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Friday, 29th May, 12.00 pm, Seminar Room
Host: Prof. Luis Liz-Marzán

Colloidally Stable, Water Soluble, Biocompatible, Semiconductor Nanocrystals with a Small Hydrodynamic Diameter

Paul Mulvaney, University of Melbourne,
School of Chemistry & Bio21 Institute

We report a simple, economical method for generating water soluble, biocompatible nanocrystals that are colloidally robust and have a small hydrodynamic diameter. The nanocrystal phase transfer technique utilizes a low molecular weight amphiphilic polymer that is formed via maleic anhydride coupling of poly(styrene-co-maleic anhydride) with either ethanolamine or Jeffamine M-1000 polyetheramine. The polymer encapsulated water soluble nanocrystals exhibit the same optical spectra as those formed initially in organic solvents, preserve photo-luminescence intensities, are colloidally stable over a wide pH range (pH 3–13), have a small hydrodynamic diameter and exhibit low levels of non-specific binding to cells.

We then demonstrate a method for conjugation based on click chemistry for linking QDs and nanocrystals to biological objects such as proteins.

Analytical Ultracentrifiugation (AUC) provides a useful tool for characterizing quantum dots and bioconjugated nanocrystals. In the final part, we describe our work on preparing CdSe based quantum dots for work in biolabelling, and the effects of ligands and coatings on their behaviour in AUC. In principle, AUC can be used to determine the stoichiometry of QD bioconjugates.

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SEMINAR

Monday, 15th June, 12.00 pm, Seminar Room

Host: Prof. Luis Liz-Marzán

Programmable Atom Equivalents from Nucleic Acid-Modified Nanoparticle Constructs

Prof. Chad A. Mirkin
Department of Chemistry and International Institute for Nanotechnology
Northwestern University
Evanston, IL 60208

The crystallographic parameters of atomic and ionic solids are fixed by the size and coordination number of their elemental building blocks, thus restricting the types of structures that can be formed. We have demonstrated that these limitations can be overcome using spherical nucleic acids (SNAs) as "artificial atoms" in nanoparticle superlattice assemblies. These three-dimensional conjugates consist of densely functionalized, highly oriented nucleic acids covalently attached to the surface of inorganic nanoparticles or proteins. The strength and length of the programmable DNA "bonds" between these nanostructures can be adjusted by varying DNA sequence and length, and the properties of the "atoms" can be adjusted by varying nanoparticle size, shape, and composition. We have developed design rules for this assembly process, analogous to Pauling's Rules for ionic solids but ultimately more powerful. These rules can be used as a guide for the rational construction of functional nanoparticle-based materials for plasmonic, photonic, and catalytic applications

CIC biomaGUNE

SEMINAR

Thursday, 25th June, 12.00 pm, Seminar Room

Host: Dr. Marek Grzelczak

Twisted Polycyclic Aromatic Hydrocarbons with Pyrazine Rings: From Molecular to Low-dimensional Materials

Aurelio Mateo-Alonso[a,b]

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Polycyclic aromatic hydrocarbons (PAHs) are receiving a great deal of attention because of their increasingly better performance in organic electronic applications. Among these, PAHs containing N atoms (N-PAHs) are particularly interesting since their electronic structure, stability, solubility, and supramolecular organization can be modulated by varying the number and position of N atoms.

In general, PAHs are planar structures but they can adopt twisted conformations as the result of the steric strain induced by overcrowding or congestion in key positions of the aromatic core. *Twisted*-PAHs have shown enhanced solubility and unique optoelectronic and chiroptical properties as an effect of their distorted molecular structure.

We have developed a general strategy that provides access to a new family of *twisted*-N-PAHs (0D) with different twist angles by introducing silyl groups with different size and rigidity, providing direct experimental correlation between twist size and properties. In addition, this methodology has been successfully implemented in the preparation of low-dimensional materials (1D and 2D). The most recent advances of these materials including synthetic routes, optoelectronic properties, self-organising properties, and potential applications will be discussed.

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CIC biomaGUNE

SEMINAR

Wednesday, 8th July, 12.00 pm, Seminar Room

Host: Dr. Niels C. Reichardt

Chemicals and Materials from Biomass

Dr. Jalel Labidi
Departamento de Ingeniería Química y del Medio Ambiente
Universidad del País Vasco

The energy crisis derived from the imminent depletion of the fossil resources and the massive dependency of these feedstocks is leading to plenty of important implications at economic, social and environmental scale. These issues evidence the need of use of other sources for energy and commodities production. In this sense, the biorefinery appears as the best solution for the sustainable obtaining of a wide spectrum of marketable products.

The main aim of our research activities is to convert lignocellulosic biomass in energy, fuels, chemicals and materials using sustainable processes.

Different lignocellulosic feedstocks, derived from agricultural, industrial and forestall activities, have been analyzed as potential raw materials for the biorefinery. Their suitability as source of value added products has been evaluated by means of the application of different pretreatment process, separation and purification techniques. The main fractions of lignocellulosic biomass (cellulose, lignin and hemicelluloses) were used to develop several applications that will be presented.

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SEMINAR

Tuesday, 14th July, 12.00 pm, Seminar Room

Host: Prof. Luis Liz-Marzán

Mediating plasmonic signature of metal nanostructures within polymer matrices

Vladimir V. Tsukruk
School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, USA

We discuss our recent results on responsive organized hybrid (polymer-nanostructures) nanomaterials, which combined from plasmonic nanostructures and encapsulated into flexible and responsive organized polymer shells and matrices. We focus on controlling, mediating, and tuning plasmonic signatures of anisotropic noble metal nanostructures with emphasis on peak appearance and shift, broadband absorption and reflection, Raman activity and control of polarization. We explore various factors such as surrounding pH, electrical field, light absorption, and magnetic field in order to control assembly of nanostructures and their interfacial interactions as well changes in ionic or dielectric environment. First, we consider noble metal nanocubes wrapped in polymer nanoshells 1 and silver nanocubes embedded in photoisomerable matrix 2, segmented gold nanorod dimers and gold-nickel dimer nanorods mediated by external magnetic field 3,4, and silver nanocubes embedded in tunable electrochemical polymers 5. Secondly, we discuss polarization-dependent broad-band light absorption and reflection 6,7,8 as well as surface enhanced Raman scattering phenomena 9,10 noble metal nanostructures assembled on engineered periodic and nanoporous templates.

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SEMINAR

Wednesday, 15th July, 12.00 pm, Seminar Room

Host: Dr. Niels C. Reichardt

Site-specific glycoproteome analysis for biomarkers in autoimmune diseases

Carlito B. Lebrilla
University of California, Davis

Immunoglobulins are abundant antibody proteins in serum that play a critical role in the active immune response. They are also highly glycosylated with varying numbers of glycosylation sites and glycoforms associated with each site. It has long been known that autoimmunity is associated with glycan changes in the serum glycome, however with the general relationships between immunoglobulins and autoimmunity has not been well explored. The limitation in determining site-specific glycosylation and quantitation of individual glycoforms has made it unfeasible to observe this relationship. In this presentation, we describe a method for extensive site-specific analysis of protein glycosylation. The glycan map of antibody proteins including IgG, IgA, and IgM is performed on a site-specific level with extensive structural heterogeneity. A mass spectrometry method, multiple reaction monitoring (MRM) is then used to quantitate glycoforms at the site-specific level. The method is used to determine the glycan changes associated with autoimmune diseases including AIDS and atopic dermatitis.

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SEMINAR

Friday, 11th September, 12.00 pm, Seminar Room

Host: Prof. Luis M. Liz-Marzán

Plasmonic Metal Oxide Nanocrystals

Delia J. Milliron
McKetta Department of Chemical Engineering, The University of Texas at Austin

Wide bandgap semiconductors such as metal oxides can be rendered plasmonic by doping to introduce exogenous free carriers. In the past few years, a number of doped metal oxides (i.e., transparent conducting oxides) have been prepared as colloidal nanocrystals. These nanocrystals have synthetically tunable doping levels, shapes, and sizes, giving rise to localized surface plasmon resonance (LSPR) absorption in the near- and mid-infrared. These new plasmonic nanomaterials may be useful for bio-sensing, photothermal therapy, and photoacoustic imaging. To explore their suitability for such applications, we have been pursuing a fundamental understanding of how doping levels, dopant distributions, shape, and composition determine their LSPR characteristics. Besides correlating optical spectroscopy with material characteristics, we are simulating the electric near fields created under infrared excitation. These simulations predict that LSPR peaks of few-nanometer diameter metal oxide nanocrystals could be more sensitive than large gold nanorods for bio-molecule detection and could effectively heat their surroundings under illumination by near infrared light that easily penetrates biological environments. Furthermore, these LSPR peaks can be modulated by charging the nanocrystals; we demonstrated that biochemical redox events can be detected optically by monitoring peak shifts.

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SEMINAR

Monday, 21st September, 12.00 pm, Seminar Room

Host: Dr. Sergio Moya

Charge regulation of hydrogels through pH and ionic strength: Implications for protein adsorption

Igal Szleifer
Department of Biomedical Engineering
Department of Chemistry
Department of Chemical and Biological Engineering
Department of Medicine
Northwestern University
2145 Sheridan Rd.
Evanston, IL 60208

The development of synthetic materials for biorelated applications requires exquisite control of the physical and chemical environment within the materials. In this talk we will discuss how charge within a hydrogel is controlled by bulk pH and ionic strength. The pH within hydrogels is very different from that of the bulk solution. The physical and chemical properties of pH-responsive gels are found to depend on the coupling between acid-base equilibrium, molecular organization and physical interactions. For example, the network's degree of protonation is not only determined by chemical composition of the bath solution but also by the ability of the polymeric structure to modify the local environment. This coupling results in swelling (or shrinking) that depends on the bath pH and salt concentration. We will discuss the gradients of protonation state and pH in hydrogel thin films that result from the inhomogeneous distribution of species within the film and how this effect has implications on the effective interactions between proteins and the film. The role of pH and ionic strength on protein adsorption and its implications to chromatography will be discussed. In particular the dramatic changes that we predict for different amino acids within the proteins when adsorbed in the hydrogel as compared to bulk solution. The theoretical predictions can be used as guidelines for the design of responsive gels in a variety of applications ranging from drug delivery systems to tissue engineering scaffolds and they provide for fundamental understanding on the non-trivial behavior of these gels. Moreover, our predictions demonstrate that the chemical state within soft materials may be dramatically different from that of the environment solutions in contact with them.

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SEMINAR

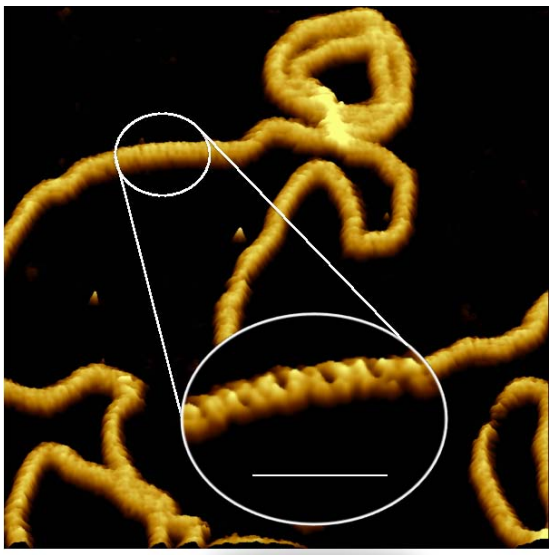
Thursday, 24th September, 12.00 pm, Seminar Room

Host: Dr. Ralf Richter

Atomic force microscopy: What we can learn from prodding biomolecules

Dr. Bart Hoogenboom
London Centre for Nanotechnology
London, UK

Life depends on intricate machinery that operates at the molecular level. I will show several examples on how we use atomic force microscopy (AFM) to prod and visualise this machinery at ~1 nm spatial resolution. This includes resolving variations of the Watson-Crick double helix structure in single DNA molecules; real-time imaging of membrane attack by bacterial toxins; and measuring and understanding the nanomechanics of polymers that determine transport into and out of the cell nucleus.



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SEMINAR

Thursday, 8th October, 12.00 pm, Seminar Room

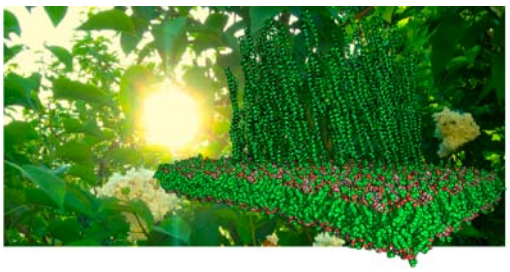
Host: Dr. Niels C. Reichardt

Protein control of soft and hard matter

Tobias Weidner
Max-Planck-Institute for Polymer Research, Mainz, Germany

Proteins can act as Nature's engineers at interfaces and manipulate both hard and soft tissue – they can shape biominerals, manipulate cell membranes and sense external stimuli. Despite the apparent importance for engineers working in the fields of implant design, tissue engineering, drug delivery, or diagnostics, the molecular mechanisms behind interfacial protein action have remained largely elusive. In order to understand protein function our goal is to probe the structure and structural dynamics of such active proteins, while they are in action at the surface. We use methods based on ultrafast sum frequency generation (SFG) spectroscopy and computer simulations to determine the structure and the mode of action by which these proteins interact with and manipulate interfaces.

Mineral proteins have the ability to control and steer the growth of biogenic hard tissue. Specialized peptides can bind and release specific mineral facets and grow the intricate mineral morphologies found in diatom cell walls, mollusk nacre, but also human teeth and bone. Taking clues from Nature we aim at understanding the mineralization processes at the molecular level and to develop design rules for biogenic nanophase materials.[1,2]



Chloroplasts are the solar cells of plants and green algae – these organelles host the photosynthesis machinery, which can convert light energy to produce biochemical energy and the oxygen we breathe. Photosynthesis takes place in a specialized structure within chloroplasts, the thylakoid membrane system. This membrane is harboring the complexes of the photosynthetic electron transfer chain. We discovered a first membrane fusion protein, IM30 (figure), involved in thylakoid membrane genesis. Using a combination of SFG, fluorescence essays and electron microscopy we have determined how IM30 binds membrane surfaces.[3]

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SEMINAR

Thursday, 15th October, 12.00 pm, Seminar Room
Host: Dr. Juan C. Mareque-Rivas

Modular Multimodal Iron Oxide-Based Nanocarriers for Image-Guided dsRNA Immunostimulation and Platinum Anticancer Drug Design

Beatriz Macarena Cobaleda
Theranostic Nanomedicine Lab

The increasingly important need for combining complementary imaging modalities and of using molecular imaging in drug development has triggered our interest in developing multimodal imaging probes which could be applied for efficient stimulation of the immune system against infectious diseases and cancer. Furthermore, the possibility of incorporating different complementary drug payloads in nanosystems could potentially lead to enhanced efficacy of conventional therapies.

The work presented in this thesis focuses on the preparation of IONP-based self-assembled nanoconstructs (iron oxide nanoparticles-filled micelles prepared from hydrophobic IONPs and PEGylated phospholipids; IONP@PL-PEG) which combine multimodal imaging capabilities with immunological and anticancer activity.[1–3] Immunological activity is induced by decorating with poly (I:C) the IONP@PL-PEG micelles; a synthetic mimic of viral double-stranded RNA (dsRNA) which has been shown to have both anticancer activity and adjuvant effects on mammalian immune responses. The anticancer activity, however, is provided by the attachment of a Pt(IV) cisplatin prodrug as a chemotherapeutic agent.

The association of poly (I:C) with a Pt(IV)-functionalized water soluble micelles provides a promising double functionalization with chemotherapy and immunostimulatory drugs in a single system.

I will also show that this pathogen-mimetic construct can be tracked *in vitro* and *in vivo* in real time using three complementary imaging modalities: fluorescence microscopy, SPECT and MRI. The combination of SPECT/MRI reveals effective lymphatic trafficking of the multifunctional nanoconstruct, which is a desirable feature for targeted chemoimmunotherapy.

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SEMINAR

Thursday, 29th October, 12.00 pm, Seminar Room

Host: Prof. Luis M. Liz-Marzán

Material-cell interactions: From TiO_2 nanoparticles to conducting polymers

Christine Payne, PhD
Associate Professor
School of Chemistry and Biochemistry
Georgia Tech, Atlanta, USA

The goal of the Payne Lab at Georgia Tech is to understand how cells and proteins interact with nanoscale materials and then use this understanding to generate new materials. This talk will focus on two new areas of research. First, we have recently determined that titanium dioxide nanoparticles, used widely in consumer products, lead to a unique oxidative stress response in human cells. Specifically, the peroxiredoxin family of anti-oxidant enzymes shows changes in gene expression following incubation with relatively low concentrations of TiO_2 nanoparticles. This response is not observed following incubation with polystyrene nanoparticles. Current research is aimed at determining the properties of TiO_2 nanoparticles that lead to this oxidative stress response. Second, we have shown that iron-containing biomolecules can be used as oxidants for the synthesis of the conducting polymer PEDOT:PSS. Recent work has examined the underlying mechanism of this reaction, with the goal of designing tunable conducting polymers by choice of biomolecular oxidant.

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SEMINAR

Tuesday, 3rd November, 12.00 pm, Seminar Room
Host: Dr. Jordi Llop

Exploring new labelling strategies for boronated compounds: towards fast development and efficient assessment of BNCT drug candidates

Kiran Babu Gona
Radiochemistry-Nuclear Imaging

Boron neutron capture therapy (BNCT) is a binary approach to cancer therapy which relies in the selective or preferential accumulation of ^{10}B atoms in the tumor; local irradiation with non ionizing thermal neutrons yields ^{4}He and ^{7}Li ions which, due to their high linear energy transfer, are able to damage tumor cells. Its clinical application has been historically restricted, mainly due to: (i) the lack of compounds able to selectively deliver boron atoms in sufficient quantity in the tumor, and (ii) the lack of techniques able to determine, *in vivo* and on real time, the accumulation of boron compounds in the tumor and surrounding tissue. In this context, nuclear imaging techniques such as PET and SPECT are valuable tools for the assessment of pharmacokinetic properties of new chemical entities

The main aim of this PhD thesis was the development of strategies for the incorporation of radioactive isotopes (mainly positron and gamma emitters) in boron rich structures (carborane clusters), to enable the subsequent preparation of a library of potential BNCT drug candidates and their evaluation using nuclear imaging techniques such as PET and SPECT in combination with anatomical techniques such as CT. With that aim, the most widely used carborane clusters, namely dicarba-*closo*-dodecaboranes and cobalt-*bis*-dicarbiollide (COSAN), were selected and strategies to radiolabel them with different isotopes such as ^{11}C, ^{18}F, ^{124}I, ^{125}I and ^{131}I were developed.