I "Julio Palacios" International Symposium

July 20th to 22nd, 2016

A Coruña, Spain

Book of Abstracts of the I "Julio Palacios" International Symposium

Edited by

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Cover:

Photograph: Julio Palacios (1916)

Picture: "Benzene" © Margarita Cimadevila

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Este simposio se enmarca en las actividades de la Cátedra “Julio Palacios”, creada en 2015 por el Consejo Superior de Investigaciones Científicas.

Julio Palacios fue un eminente científico y humanista español, y el objetivo de este evento es poner en valor su figura y ofrecer un punto de encuentro divulgativo sobre las fronteras actuales de las ciencias naturales, aspecto al que presta mucha atención la Universidad de A Coruña (UDC).

En este documento se recogen las actividades desarrolladas durante los tres días de celebración del evento, actividades que incluyen conferencias, las cuales abarcan diversos campos científicos y académicos en los que trabajó Julio Palacios, comunicaciones tipo póster y una mesa redonda, todo ello de carácter multidisciplinar.

El comité organizador quiere agradecer la primordial financiación de la FUNDACIÓN RAMÓN ARECES, así como la aportación de la Universidade da Coruña y el apoyo recibido por la Real Sociedad Española de Matemáticas (RSEM) y el Consejo Superior de Investigaciones Científicas (CSIC).

Julio Palacios Martínez (1891-1970) nace en Paniza (Aragón) el 12 de Abril de 1891. Obtiene su licenciatura en Ciencias Exactas y Físicas en 1991 en Barcelona con premio extraordinario.

Realiza su tesis doctoral en Madrid bajo la dirección de Blas Cabrera, director del Laboratorio de Investigaciones Físicas (LIF) de la Junta para Ampliación de Estudios (JAE), presentándola en 1914 y obteniendo también el premio extraordinario.

En 1916 obtiene por oposición, la cátedra de Termología en la Universidad Central de Madrid. Después de lo cual se desplaza a la Universidad de Leiden (Holanda), para trabajar con H. Kamerlingh Onnes en Leiden (Holanda) –descubridor de la superconductividad–. Allí asiste a los cursos de Física Teórica de Lorentz y a los coloquios físico-matemáticos de Ehrenfest, publicando una serie de artículos que serían el inicio de su carrera científica y académica.

De vuelta a España ejerce como docente en la facultad de Ciencias de la Universidad Central de Madrid y continúa sus investigaciones en el LIF. En 1923 participa en la preparación de los actos y conferencias de la visita de Albert Einstein a España, y en 1927 forma parte de la Junta Constructora de la Ciudad Universitaria de Madrid.

Su labor científica y académica transcurre entre el Instituto Nacional de Física y Química, dirigiendo la sección de Rayos X, y la Universidad Central de Madrid.

Finalizada la Guerra Civil, se reincorpora a la cátedra de Termología en Madrid, y entre 1947 y 1961 su vida transcurre entre esta ciudad y Lisboa, dirigiendo a nuevos grupos de investigación, y dedicándose esencialmente a escribir libros con los que estudiaron varias generaciones de científicos españoles.

Durante esta etapa se interesa por temas biológicos desde la perspectiva de la Física, siendo nombrado director de la sección de Física del Instituto de Oncología de Lisboa, alternando la docencia entre esta ciudad y Madrid.

La obra escrita de Palacios comprende 14 libros y 163 publicaciones científicas. En 1922 traduce del alemán las obras de Planck (Termodinámica), Reiche (Teoría de los quanta: su origen y desarrollo) y Eichwald (Los fundamentos físico-químicos de la Biología). Palacios ocupa la cúspide mundial durante muchos años en el *Análisis Dimensional*, su obra más conocida y traducida a distintos idiomas. Cabe destacar también su obsesiva oposición a la teoría de la relatividad de Einstein.

Palacios destaca como humanista en el sentido clásico, llegando a ser miembro de distintas academias, y Presidente de la Real Academia de Ciencias Exactas, Físicas y Naturales, desde 1966 hasta su muerte en 1970 en Madrid. De su matrimonio con Elena Calleya Pedroso, nacen cinco hijas: Elena, Carmen, Pilar, Ana María y María del Rosario.

Información más detallada sobre la vida y obra de Julio Palacios se puede consultar en:
Julio Palacios Martínez (1891-1970): Un científico entre la física y la química
Josep Mª Oliva
An. Quím. **2013**, *109*(2), 106 – 109
http://analesdequimica.es/index.php/AnalesQuimica/article/view/65/63

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La Fundación Ramón Areces está orientada desde su constitución en 1976 al mecenazgo científico, mediante el fomento de la investigación, la contribución a la generación de capital humano y la difusión del conocimiento.

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Program

Wednesday, 20th July 2016

18:00 – 18:30 *Opening ceremony*

18:30 – 19.15 Albino Arenas, UPM

- Julio Palacios: recuerdos de un maestro / *Julio Palacios: Memories from a master*

19:15 – 20:00 Francisco González de Posada, UPM

- Julio Palacios: Relatividad y análisis dimensional / *Julio Palacios: Relativity and dimensional analysis*

Thursday, 21st July 2016

9:00 – 10:00 *Registration*

Chair*: Philip Mayles*

10:00 – 10:45 Helen Mayles, *Clatterbridge Cancer Center*, UK

- *Harnessing X-Rays to treat cancer – Challenges in modern radiotherapy physics*

10:45 – 11:30 Maria Paula Diogo, *Universidade Nova de Lisboa*, Portugal

- *Julio Palacios: Balancing science and politics during the portuguese dictatorship*

11:30 – 12:00 *Pause*

Chair*: J. Arturo Santaballa*

12:00 – 12:45 Fernando Martín, *UAM*, Spain

- *Attosecond light: The superslow-motion camera of physics, chemistry and biology*

12:45 – 13:30 Juan Hermoso, *CSIC*, Spain

- *X-ray crystallography: Exploring the life at atomic level*

13:30 – 16:00 *Pause*

Chair*: José I. Burgos Gil*

16:00 – 16:45 Pilar Bayer, *University of Barcelona*, Spain

- *Fourier coefficient estimates of automorphic forms: known results and conjectures*

16:45 – 17:30 William Seitz, *Texas A&M University*, USA

- *A new relationship between complexity and entropy*

17:30 – 18:00 *Pause*

Chair*: Ricardo Cao*

18:00 – 18:45 Ángel Carracedo, *Institute of Forensic Sciences, USC*, Spain

- *The genomic revolution*

18:45 – 19:00 Margarita Cimadevila

- "Avant-garde in science" exhibition

19:00 - 20:00 *Poster session*

Friday, 22nd July 2016

Chair*: Gerardo Delgado-Barrio*

9:15 – 10:00 Ignacio Cirac, *Max Planck Institute for Quantum Optics*, Germany

- *On the difficulty of simulating complex quantum systems*

10:00 – 10:45 Daniel Roca-Sanjuán, *University of Valencia*, Spain

- *Chemistry, light, and computers*

10:45 – 11:15 *Pause*

Chair*: Moisés Canle*

11:15 – 12:00 José I. Burgos Gil, *CSIC*, Spain

- *Can you tell if a number is new?*

12:00 – 12:45 Douglas Klein, *Texas A&M University*, USA

- *Partial orders: Substitution reactions*

12:45 – 13:30 Javier Brey, *University of Sevilla*, Spain

- *Granular matter: a biased overview*

13:30 – 16:00 *Pause*

Chair*: Douglas J. Klein*

16:00 – 16:45 Eluvathingal Jemmis, *Indian Institute of Science*, Bangalore, India

- *Importance of early questions*

16:45 – 17:30 Harald A. Helfgott, *Georg-August Universität Göttingen, Germany, and CNRS,* France

- *The ternary Goldbach conjecture*

17:30 – 18:00 *Pause*

Moderator: Gerardo Delgado-Barrio

18:00 – 19:30 *Multidisciplinar round table*

19:30 – 20:00 *Closing ceremony*

Keynote talks

Julio Palacios: recuerdos de un maestro

Albino Arenas
Escuela Universitaria de Ingeniería Técnica Industrial,
Universidad Politécnica de Madrid, 28012 Madrid
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Julio Palacios fue presidente de la Real Academia de Ciencias Exactas, Físicas y Naturales y miembro de la Real Academia de la Lengua y de la Real Academia de Medicina. Era catedrático de la Facultad de Ciencias de la Universidad Central de Madrid (actualmente Complutense). Fue uno de los pioneros de la investigación en física en nuestro país. Trabajó con el premio Nobel de Física Kamerlingh Onnes con el que publicó dos artículos científicos. Participó en los actos de homenaje que se le rindieron a Einstein en su visita a Madrid en 1923. Autor de numerosos artículos de investigación y libros, destaca, entre estos, "Análisis Dimensional", traducido al inglés y al francés, primer libro escrito por un físico español merecedor de tal distinción.

Albino Arenas, último discípulo directo de Julio Palacios, realizará una pequeña semblanza biográfica de su figura y relatará algunos de los recuerdos del que fuera referente y maestro de la física española durante varios decenios: Julio Palacios.

Y, juntamente con ello, expondrá algunas de las circunstancias que lo convirtieron en una figura de relevancia pública en la vida española.

Julio Palacios: Memories of a Master

Albino Arenas
Escuela Universitaria de Ingeniería Técnica Industrial,
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Julio Palacios was the President of the Royal Academy of Exact, Physical and Natural Sciences (Real Academia de Ciencias Exactas Físicas y Naturales) and member of the Royal Academy of Language (Real Academia de la Lengua) and the Royal Academy of Medicine (Real Academia de Medicina).

He was Professor at the Faculty of Sciences at the Central University of Madrid (Universidad Central de Madrid), now with the name of Complutense University of Madrid (Universidad Complutense de Madrid). Palacios was one of the pioneers in Physics research in Spain. He worked with the Nobel Prize of Physics Kamerlingh Onnes and published two papers with him. Julio Palacios took part in the tribute acts that Einstein received during his visit to Madrid in 1923. He is author of a lot of scientific articles and books. Among the books, it should be pointed out *"Dimensional Analysis"* (*Análisis Dimensional*), translated to English and French. It is the first book written by a Spanish Physicist that has deserved such distinction.

Albino Arenas, the last direct disciple of Julio Palacios, will make a small biographical sketch. He will relate some of the memories of Julio Palacios, which was a model and master for the Spanish Physics for several decades. And, together with it, he will present some of the circumstances that turned him into a prominent figure in the Spanish public life.

Julio Palacios: Relatividad y Análisis Dimensional

Francisco González de Posada
Universidad Politécnica de Madrid
francisco.gonzalez@upm.es

Julio Palacios ha pasado a la historia de la ciencia española por su dedicación y papel desempeñado en los siguientes ámbitos objeto de reflexión.

Primero. Escritor excepcional de libros de texto de numerosas ramas de la física.

Segundo. Ocupar la cúspide mundial en Análisis Dimensional.

Tercero. Obsesiva oposición a la teoría de la relatividad de Einstein.

Cuarto. Filósofo de la ciencia física.

Julio Palacios: Relativity and dimensional analysis

Francisco González de Posada
Universidad Politécnica de Madrid
francisco.gonzalez@upm.es

Julio Palacios has passed through history of Spanish science for his dedication and rôle played in the following issues.

First. Exceptional writer of text books in several branches of physics.

Second. Occupy the world cusp in Dimensional Analysis.

Third. Obsessive oposition against Eintein's Theory of Relativity.

Fourth. Philosopher in physics.

Harnessing X-Rays to treat cancer – Challenges in modern radiotherapy physics

Helen Mayles, MSc
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Helen.Mayles@clatterbridgecc.nhs.uk

Although, he would not have called himself a medical physicist, my grandfather had many of the characteristics of those early pioneers in medical physics: University radiation physicists who worked with clinical colleagues in setting up hospital departments, used for the diagnosis and treatment of cancer. He died when I was a young teenager but he had influenced me to the extent that, having read physics at university. I embarked on a career as a Medical physicist. My first jobs were in London, then in 1994 I moved to the Clatterbridge Cancer Centre that serves the population of Liverpool and surrounding area.

Radiotherapy started when it was seen that radium needles could sterilise tumours when placed inside or adjacent to them for a specified time. Called brachytherapy, this type of treatment is still used for the skin and inside body cavities, but it is not practical for inaccessible deep seated tumours. It was soon followed by Cobalt-60 machines which directed the high energy gamma rays produced by radioactive decay into useable beams. Eventually the modern linear accelerator was developed. With this machine, X-ray beams can be shaped so that a high dose is given to the tumour while sparing the surrounding normal tissues. Tumours and normal tissue are identified using modern imaging techniques which enable one to "see" inside the body, such as magnetic resonance imaging (MRI) and computer tomography (CT). Together with surgery and chemotherapy, radiotherapy is a vital tool in treating cancer.

My talk will illustrate how imaging is used to identify tumours and normal tissues, and how "treatment plans" are created using computer models of linear accelerator beams and algorithms that predict how these beams impart energy to human tissue. I will address the challenges of treating small tumours in sensitive organs, such as the brain, and tumours that move, such as in the lung. I will show that physicists are a essential part of the team, continuously improving the effectiveness of radiotherapy treatments.

Julio Palacios: balancing science and politics during the Portuguese dictatorship

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Julio Palacios moved from Spain to Portugal during a particularly difficult moment for the two Iberian dictatorships. In the aftermath of World War II, the victory of the Allies shook both Franco's and Salazar's regimes and gave those who opposed them a glimpse of hope. This optimism proved wrong. Reacting to the new framework of the Cold War, both dictators strengthened their political surveillance and repression, thus persecuting all those who could be accused of socialist or communist leanings and conspiracy.

In Portugal, the Laboratory of Physics of the Faculty of Sciences of the University of Lisbon, directed by Manuel Valadares, suffered a severe blow when three of its researchers, including Valadares, were accused of subversive activities and dismissed from the academia.

Julio Palacios, Full Professor and Vice-Dean of the University of Madrid, was suggested by the Dean of the Faculty of Sciences of the University of Lisbon as the right man to occupy Valadares' post. However, the new position turned out to be a thorny path. Although Palacios used to visit regularly the Laboratory of Physics and held in high esteem its researchers, he was received coldly when he took the lead.

Despite theses difficulties, Julio Palacios managed to implement a set of research programs and to balance his scientific and political sympathies, thus becoming a key actor in the scientific millieu of the postwar period in Portugal.

Attosecond light: the superslow-motion camera of physics, chemistry and biology

Fernando Martín
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The advent of attosecond light pulses has opened new avenues for imaging electronic and nuclear dynamics in molecules, with exciting applications in physics, chemistry and biology. Processes such as ionization, ultrafast charge migration, proton transfer, or isomerization can now be monitored in their natural time scale. Such progress would not have been possible without the help of theoretical modeling. In this talk, the history of this joint venture and its future implications will be discussed.

X-Ray crystallography: Exploring the life at atomic level

Juan A. Hermoso
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Along its 100 years of existence crystallography has become the leading technique for studying the atomic structure of materials and is the center of advances in many fields of science, such as Physics, Chemistry, Condensed matter, Biology or Biomedicine. X-Ray crystallography opened a window to the molecular world unraveling the extraordinary complexity, and beauty, hidden in the inorganic and living things.

Thanks to the structural knowledge provided by crystallography, today we are able to produce new materials and to develop new products in aeronautic, automobile, pharmaceutical, computer among others.

Crystallography helps to reveal some of the mysteries of the structure of life by knowing the atomic structure of the key players of the life: the proteins. Structures of proteins and nucleic acids are vital for elucidating protein functions and intermolecular interactions and for improving understanding of basic biological and biochemical mechanisms and disease pathways. Their immediate practical application is in the design of pharmaceuticals, in which they play a central role in drug discovery.

Along this talk the basics of crystallography, its legacy and future growth areas will be described together with our most recent advances in understanding a fascinating field of life: the mechanisms of bacterial infection and how we can fight against the challenge of antibiotics resistance.

Fourier coefficient estimates of automorphic forms: Known results and conjectures

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Throughout history, many results of an arithmetical nature have been proven by means of analytic tools, such as those provided by zeta and L-functions. But the inverse statement is no less true: algebraic and geometric results can also lead to analytic results, as was evidenced by the research emanating from some of the most famous Ramanujan conjectures.

The talk will focus on automorphic forms and will show some of the links discovered between arithmetic and analysis, in order to acquire a better understanding of "numbers". Endowed with a differential factor, the concept of automorphic form generalizes that of a periodic function. Automorphic forms are present in almost every area of modern number theory and there is a widespread belief that all L-functions occurring in number theory and arithmetic algebraic geometry should be automorphic.

Automorphic forms also appear in other areas of mathematics, such as representation theory or harmonic analysis, and in mathematical physics.

A new relationship between complexity and entropy

William A. Seitz
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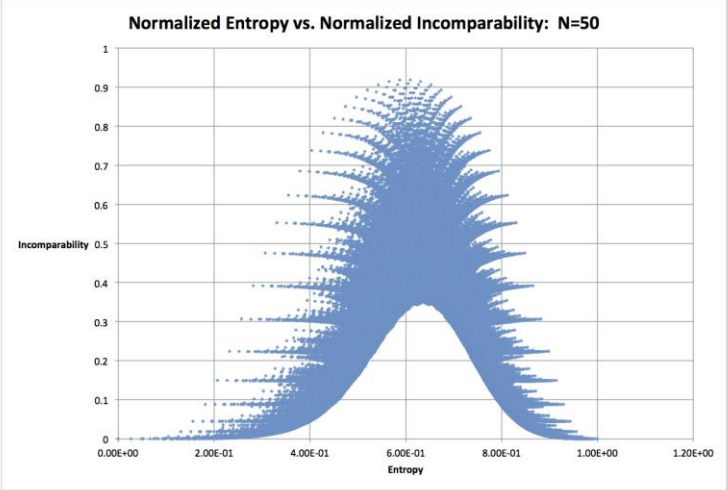
While entropy appears to be well defined in science, the term complexity is not. The talk will first define complexity in a quantitative sense for Boltzmann statistics and show how complexity and entropy are related. For a preview of this, see the figure below showing complexity as a function of entropy for this system.



The talk will continue to explore this complexity view qualitatively in a large number of systems all of which are characterized as being partially ordered. Systems to be discussed are genes, organizations, ecosystems, urban planning, social organizations, and others. Evolution from very ordered systems, (initially with low entropy), to disordered systems with high entropy shows complexity initially increasing with time, followed by ultimate decay. These observations have important consequences for sustainability.

The genomic revolution

Ángel Carracedo
Instituto de Ciencias Forenses. Univesidade de Santiago de Compostela
Fundación Pública Galega de Medicina Xenómica (SERGAS)
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The completion of the human genome project in 2002 and the launch of numerous international projects in genomics have caused a revolution in many areas of medicine. Inheritable genetic diseases can be diagnosed in a large percentage because we know the genes responsible for most. The introduction of massive genotyping and new generation sequencing technologies and the progress in the analysis of big data is now allowing the discovery of the genes involved in complex (common) disease where genetic and environmental factors interact. As a consequence diseases and patients can be stratified opening a new area of personzalized medicine.

But the genomic revolution not only influences clinical medicine, but many other areas of science: veterinary, agriculture, forestry or many other more specific sciences such as forensic medicine. Now we can not only identify individuals from mínimum amount of biological materials but even to predict physical properties such as the colour of the eyes or skin, the geographical origin of the individual or even age. This is going to be examplified to some recent cases where we have been involved such as the 11-M Madrid bomb attacks, the Minstead operation in the UK and the Eva Blanco murder case.

AVANT-GARDE IN SCIENCE
Exhibition

Margarita Cimadevila
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Throughout history, women working in the field of science had to overcome all kinds of obstacles and disadvantages to be able to study and to investigate, mostly in bad conditions. AVANT-GARDE IN SCIENCE is an homage to the courage of men, who raised themselves above the small-mindedness of their contemporaries by incorporating women into the world of Science, like Hilbert, Rutherford, Severo Ochoa and Mittag-Leffler. It is a work about women and men who were in the Avant-Garde of both, Science and Life.

The exhibition AVANT-GARDE IN SCIENCE of Margarita Cimadevila (painter and science teacher) is combining Science and Art and consists of paintings, which were inspired by the scientific work of these women and men, and of short information on their scientific achievements and life. After CIENCIA EX AEQUO [1], it is her second exhibition, which tries to make visible the role of women in Science and to fight for gender equality in Science and Life.

Rutherford´s experiment

[1] M. Cimadevila, *CIENCIA EX AEQUO*. A. López Díaz (Edición), Universidade da Coruña, A Coruña (Spain), 2013.

On the difficulty of simulating complex quantum systems

J. Ignacio Cirac
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In general, it is very hard to describe many-body quantum systems, like high-temperature superconductors, magnetic materials, chemical compounds, or those appearing in high-energy physics. This fact is mainly due to the proliferation of parameters when the number of particles increases. Quantum simulators offer an alternative to traditional methods used for this purpose, as they can circumvent some of the problems related to this explosion in the number of parameters by using a system that itself evolves according to the laws of quantum physics. In this talk I will review the idea of quantum simulation, and explain current attempts to build such equipments based on trapped atoms and ions.

Chemistry, light, and computers

Daniel Roca-Sanjuán
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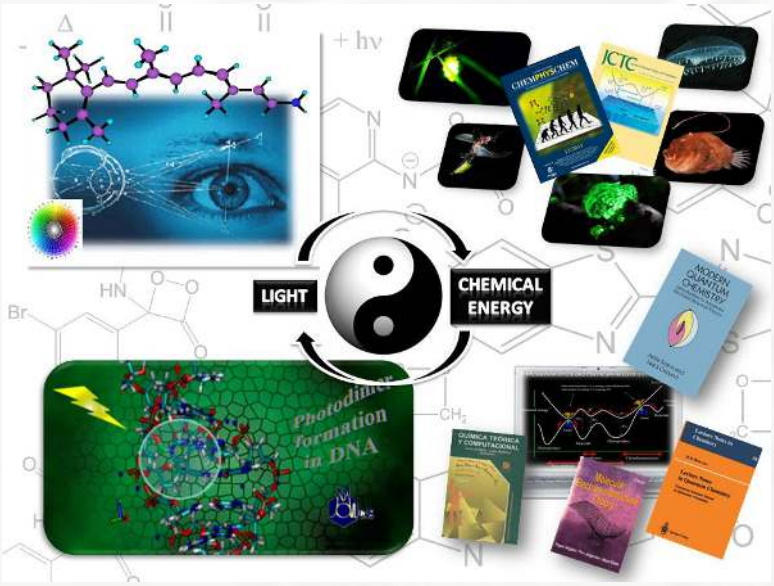
Chemistry is a beautiful branch of Science related to the properties of substances and the changes that they undergo. When matter is irradiated with light, some special transformations may take place, which are so-called photo-chemistry. This type of chemistry is responsible for crucial phenomena of Life, such as the photosynthesis, the synthesis of vitamin D, or the process of vision. Nature also presents many examples of conversion between light and chemical energy that go in the other direction, i.e., chemical reactions that give rise to light. We can find some wonderful examples in the biosphere: worms, bugs, and deep-sea creatures that produce bioluminescence for several purposes such as communication, mating, or to escape from predators. Since immemorial times, humans have tried to understand the phenomena of light-matter interaction and make use of them in their life, in some cases emulating the biological organisms. The present talk shall give an overview of the chemistry behind light-matter interactions. Moreover, illustrative examples will be provided on how computers allow a deep comprehension of the photo-chemical mechanisms and help to design new light-based technologies.



Can you tell if a number is new?

José I. Burgos Gil
Instituto de Ciencias Matemáticas (CSIC), Cantoblanco, 28049 Madrid
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As a result of a computation we may obtain a number in the form of a series, a special value of a function, an integral etc. For theoretical and practical purposes is important to know if this number is new or it can be related to known numbers.

In this talk we will give a survey on the classification of numbers: rational numbers, algebraic numbers, transcendental numbers, periods... and explain some known results and conjectures, taking as guiding example the values of the famous Riemann zeta function at integer arguments.

Partial orders: substitution reactions

Douglas J. Klein
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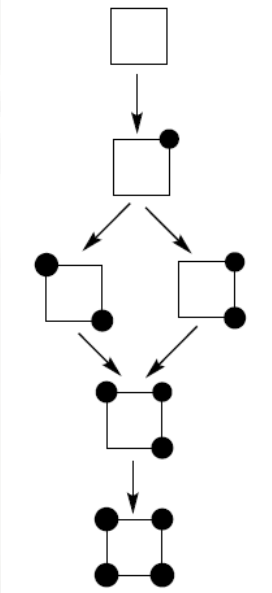
Partial orders allow a general way to make systematic comparisons. Now & again one encounters a characteristic to which various investigators ascribe different sets of numerical values – *e.g.*, for: various “bioactivities”, or chemical "aromaticity", or “symmetry”, or “complexity”. There may be numerical ambiguity imagined to be due to a conceptual "short-coming" which if only rectified by a correct definition would give "true" numerical values. But instead the characteristic may be non-numerical – not totally ordered. The various ascriptions of numerical values by different investigators would be just different partly faithful representations of an underlying "partial order" – a fundamental and useful concept complicit throughout much of science.

We recall the mathematical idea of a partially ordered set (or poset), and then illustrate it. Substitution posets provide one broad example – a specific case being that for substitution of the four ligand positions of a square-planar complex, whence the substitution poset is representable as



Hemoglobin has four such sites for attachment of O_2, though in fact the complex is of lower symmetry, so that the more exact substitution network is a little more involved.

Granular matter: A biased overview

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Granular matter is ubiquitous in Nature. It can be roughly defined as composed by a large number of macroscopic particles whose interactions are inelastic, i.e they do not conserve kinetic energy. It includes systems like the contents of a sugar bowl, the sand of a beach, an avalanche, the grains in a silo, or the Saturno rings. As granular systems are composed by many particles, it seems quite natural to extend the methods developed for molecular fluids and solids in order to describe the behavior of granular matter. Nevertheless this task has turned out to be much more complex than expected, requiring the revision of many concepts and ideas that were supposedly well established in Physics.

One aspect of granular systems rendering them very appealing for scientists is the relative easiness of performing experiments. Some features, e.g. hydrodynamic instabilities, very hard to observe in molecular systems can be easily observed with the naked eye in a system of grains. Besides, the latter exhibits a variety of peculiar behaviors quite different from those of ordinary systems.

In the talk, a short and necessarily superficial overview of this relatively young field of science will be provided, putting especial emphasis on some of the most relevant open questions, from the perspective of the fields present in this course.

It must be kept in mind that there are many basic features that are far from being scientifically understood. One of the reasons for this is that granular systems are by definition far from equilibrium, while most of the existing physics for macroscopic systems, in the sense of being composed by many particles, refers to equilibrium situations or “close” to them. From this perspective, granular systems are also a proving ground for nonequilibrium physics.

Importance of early questions

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My presentation will give emphasis to two aspects. First is that we should encourage youngsters to ask questions at an early stage. In the school, in the college much before they start research. These will generate more general and important questions. So educational system at the School and at the beginning stages of the university education must make sure that the students look at everything around and ask questions. These may be trivial or profound, but the habit must begin early. The question for which they do not get immediate answers is what propels the mind, pushes the frontiers further. A second aspect is to see the advantage of knowing several areas of study in solving important problems and advancing knowledge. Some examples from my own work will be presented to exemplify these ideas.

The ternary Goldbach conjecture

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The ternary Goldbach conjecture (1742) asserts that every odd number greater than 5 can be written as the sum of three prime numbers. Following the pioneering work of Hardy and Littlewood, Vinogradov proved (1937) that every odd number larger than a constant C satisfies the conjecture. In the years since then, there was a succession of results reducing C, but only to levels much too high for a verification by computer up to C to be possible. I have managed to give a full proof of the conjecture; we will go over the main ideas in the proof and a sketch of its history.

Poster communications

The role of upper excited states in the laser performance of *anti*-$B_{18}H_{22}$, the first laser borane

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Emission from electronically excited species forms the basis for an important class of light sources, that of lasers. So far, commercially available solution-processed blue-emitting laser materials are based on organic compounds or semiconductor nano-crystals that have significant limitations; either low solubility, low chemical- and/or photo-stability, and/or uncompetitive prices. We recently reported [1] a novel and competitive alternative to these existing laser materials that is based on the boron hydrides; inorganic cluster compounds with a rich and diverse chemistry. We have demonstrated that solutions of the borane *anti*-$B_{18}H_{22}$ show, under pulsed excitation, blue laser emission at 406 nm with efficiency (ratio of output/ input energies) of 9.5 %, and a photostability superior to many of the commercially available state-of-the-art blue laser dyes.

Although this demonstration opened the doors to the development of a whole new class of laser materials based on a previously untapped resource for laser technology -the boranes- there are still issues in its performance that hinder full commercial exploitation. For example, it is quite surprising that *anti*-$B_{18}H_{22}$, a compound with a superior quantum yield of 0.97, renders laser efficiencies lower than DPS, an organic dye with a quantum yield of 0.74.

To understand this contradiction, we have looked for the presence of several sources of losses and photophysical processes that are known to reduce the laser efficiency in this kind of systems. Among them, the excitation of upper excited states becomes most relevant, resulting not only in the lost of laser efficiency, but in the activation of chemically reactive deexcitation pathways. In this communication, apart from revisiting the laser performance of *anti*-$B_{18}H_{22}$, we will describe and quantify the sources of losses that affect this first laser borane, and will discuss their implications in its photochemistry. The use of UV/Vis absorption spectroscopy, Nuclear Magnetic Resonance spectroscopy, as well as Mass Spectrometry, allows gaining an insight into the photoproducts that are created upon high intensity laser irradiation of boranes, and shine a light on how they are formed. These results will eventually help delineating what boron chemists should look for in order to mitigate deficiencies and boost the laser efficiency and photostability of the next generation of laser boranes.

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Evidence of discs around pulsars

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Pulsars are fast rotating neutron stars, which are known to be one of the possible remnants of supernovae. Consequently, any object orbiting them should have been destroyed in the explosion. But, unexpectedly, the first extrasolar planet was found around a pulsar [1].
In spite of the discovery of hundreds of extrasolar planets in the last years, there are still just a few related to pulsars (only 5 confirmed cases orbiting 3 different pulsars) [2,3,4]. In order to explain this special kind of planetary systems, the existence of an accretion/debris disc around the neutron star was postulated [5]. These discs can be found through the study of infrared excesses in Spectral Energy Distributions (SEDs). Its presence may suggest the existence or the formation of planets around pulsars (as it also happens around "normal" stars).
Some discs have been discovered in the last years but there is still a lot to be done. The satellite WISE, with its mapping of the whole sky in the infrared, has been revealed as a useful tool for studying SEDs. Previous comparisons with Spitzer quality data provided us with a useful recipe to exploit the WISE catalogue in order to find reliable excesses and, thus, discs.

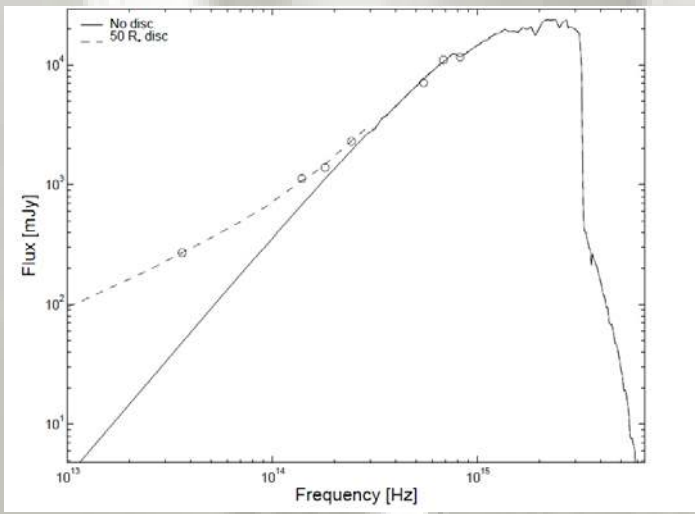

Fig.1 SED and theoretical model of the pulsar PSR B1259-63/SS 2883 [6]

After analyzing all the pulsars known to date, our results confirm previous findings and suggest that more sensitivity at these wavelengths should be needed.

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Smoothed stationary bootstrap and smoothed moving blocks bootstrap for bandwidth selection in density estimation with dependent data

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Smoothed versions of the stationary bootstrap [1,4] and moving blocks bootstrap [2,3] are established for the purpose of bandwidth selection in density estimation for dependent data. The exacts expressions for the bootstrap version of the mean integrated squared error under dependence are obtained in both contexts. Those expressions are very useful since implementation of the bootstrap selector does not require Monte Carlo approximation. A simulation study is carried out to show the good practical performance of both new bootstrap bandwidth selectors with respect to other existing competitors. The method is illustrated by applying them to two real data sets.

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Nonparametric Inference for big-but-biased data

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Crawford [1] has recently warned about the risks of the sentence "with enough data, the numbers speak for themselves". Some of the problems coming from ignoring sampling bias in big data statistical analysis has been recently reported by Cao [1]. The problem of nonparametric statistical inference in big data under the presence of sampling bias is considered in this work. The mean estimation problem is studied in this setup, in a nonparametric framework, when the biasing weight function is known (unrealistic) as well as for unknown weight functions (realistic). In the latter setup the problem is related to nonparametric density estimation. Asymptotic expressions for the mean squared error of the estimators proposed are considered. This leads to some asymptotic formula for the optimal smoothing parameter. The question of how big the sample size has to be to compensate the sampling bias in big data is considered. Some simulations illustrate the performance of the nonparametric methods proposed in this work.

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Acoustic characterization of a viscoelastic tile using frequency-dependent ultrasound measurements

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At ultrasound frequencies, polymers show a viscoelastic mechanical behaviour [1]. The choice of a suitable viscoelastic model is fundamental in any numerical procedure on computational acoustics to get a mechanical response as accurate as possible in comparison with the experimental data. Well-known viscoelastic material models such as Maxwell and Kelvin-Voigt models [2] or the more recent fractional derivative viscoelasticity models [3] are common model assumptions for modelling linear wave propagation in viscoelastic materials.
Usually, once the frequency-dependent constitutive model is fixed, their unknown parameters are estimated to fit the experimental data with the response of the mathematical model. However, in this work, the choice of the viscoelastic model is not based on imposing any functional dependency of the parameters in terms of the frequency but only on the ultrasound experimental measurements. Hence, this approach avoids the epistemic uncertainty of a priori unsuitable model selection. The proposed technique involves the numerical computation of an inverse problem (based on the acoustic propagation of plane waves in multilayer media) at each frequency of interest. In these numerical simulations, the non-planar directivity pattern of the acoustic transducer has been considered. This methodology on the selection of the viscoelastic model is illustrated using a polyurethane tile [4] and echo reduction ultrasound measurements in an underwater environment.

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Nonparametric estimation in mixture cure models applied to colorectal cancer patients

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Current cancer treatments caused an increased ratio of cured patients or, at least, a long term survival. In order to accommodate the insusceptible proportion of subjects, a cure fraction can be explicitly incorporated into survival models and as a consequence, cure models arise. The goals in cure models are usually to estimate the cure rate (incidence) and the probability of survival of the uncured patients up to a given point of time (latency). A completely nonparametric approach for mixture cure models is introduced, as an alternative to the current parametric and semiparametric methods in the literature. Both the nonparametric incidence estimator by [4] and the nonparametric latency estimator by [2] are presented. These estimators, which are based on the Beran estimator of the conditional survival function, [1], are proved to be the local maximum likelihood estimators. An iid representation for the nonparametric incidence (latency) estimator is obtained in [2] ([3]). The choice of the corresponding optimal bandwidths is addressed by a bootstrap selection method, which behavior is assessed in a simulation study.

Finally, as a result of the cooperation of the research group MODES with the University Hospital of A Coruña (CHUAC), the proposed methods are applied to a database of colorectal cancer in CHUAC patients to determine the prognosis based on, among other variables, the age.

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Design of cyclometallated palladium (II) compounds whit unusual structure

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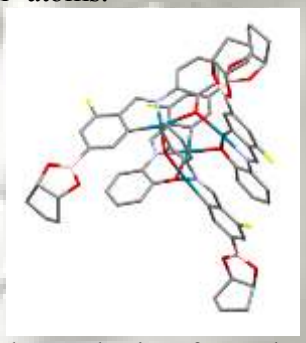
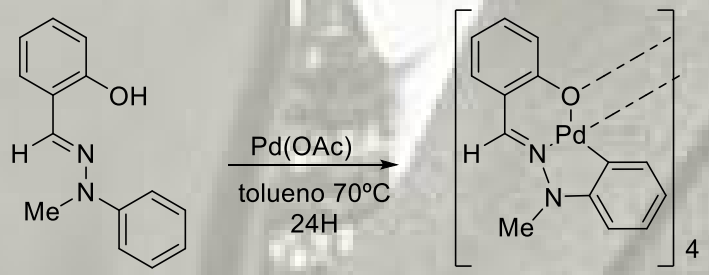
In the past, we have been interested in palladium(II) cyclometallated complexes derived from [C,N,X] (X: O, S) terdentate ligands. In the case of the terdentate [C,N,S] thiosemicarbazones and [C,N,O] imine phenol derivatives, the cyclometallation reaction gives palladium(II) derivatives, which show tetranuclear structures, with an eight membered Pd_4X_4 core (X: O, S). In order to achieve neutrality, the ligand is usually deprotonated in the complex at the hydrazinic nitrogen or the phenolic oxigen atoms.



In the present abstract we report the synthesis of a cyclometallated complex derived from N-methylhydrazone with the ligand coordinated in a [C,N,O] terdentate fashion. Reaction of 2-$OHC_6H_4C(H)=NN(Me)(C_6H_5)$ (**a**) with palladium(II) acetate in toluene at 70 ºC gave the tetranuclear cyclometallated complex [Pd{2-$(O)C_6H_4C(H)=NN(Me)(C_6H_5)$-*C2*}$_4$] (**1a**) which was fully characterized by elemental analysis (C, H, N), conductivity measurements, mass spectrometry, IR and N.M.R. (^{1}H and ^{13}C-{^{1}H}) spectroscopy and by X-ray crystallography.



a **1a**

The new compound was also characterized by X-ray crystal structure analysis. Crystals of [Pd{2-$(O)C_6H_4C(H)=NN(Me)(C_6H_5)$-*C2*}{2-$(Ph_2P)C_6H_4CHO$-*P,O*}$_4$] were monoclinic with $a = 21.705(5)$ Å, $b = 19.314(5)$ Å, $c = 14.646(5)$ Å , $\beta = 115.405(5)°$, $U = 5546(3)$ Å^3, space group = C2/c. The final refinement converged at $R_1 = 0.0244$ (observed data) $wR_2 = 0.0824$ (all data, F^2).

Noncommutative geometry and Hopf algebras

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Noncommutative algebra and geometry [1] provide an appropriate framework to formulate mathematically various phenomena of quantum physics. The formulation of quantum mechanics given by Born, Heisenberg, and Jordan at the beginning of last century needed noncommutativity. Nowadays we find ideas of these two areas, for instance, in the quantum Hall effect and the standard model. The noncommutative standard model proposed by Connes and collaborators in [2] predicted, among other things, a mass of the Higgs boson of around 170 GeV.

The purpose of this work is twofold:

On the one hand, we intend to spread some ideas of noncommutative algebra and geometry, specially, the structure of Hopf algebra, which is our research topic. Hopf algebras play here the role of groups in classical geometry in describing symmetries. We will emphasize a prominent class of Hopf algebras, the quantum groups [3] discovered by Drinfeld and Jimbo in their study of quantum integrable systems.

On the other hand, we will present several results on Hopf algebras with integral (also called co-Frobenius) [3,4], obtained by Andruskiewitsch et al. [6] and the authors [7]. In [6] a method to construct co-Frobenius Hopf algebras was developed and successfully applied to lifting of quantum lines over abelian groups [8]. The new examples so constructed allowed to answer in the negative the question posed in [9] as to whether a co-Frobenius Hopf algebra is finitely generated over its Hopf socle. Moreover, these are the first examples of noncommutative infinite-dimensional co-Frobenius Hopf algebras fitting in an exact sequence with finite-dimensional kernel and cosemisimple cokernel. This fact forced to change the ideas handled so far about the form of this kind of Hopf algebras.

Our current research [7] is addressed to check the validity of that method on lifting of quantum lines over non-abelian groups. Our study on dihedral and quaternion groups has revealed a way of deforming the previous examples and we can now elucidate the form of the examples that will be obtained when applying the method to any finite group.

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Design of new Ru(II) polypyridyl complexes with potential anticancer activity

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Nowadays the cancer cause a huge number of deaths in the world, and the number of global cancer deaths is projected to increase 50% until 2030[1]. In the last years, research in the design of anticancer compounds field was committed to ruthenium compounds motivated by promising results obtained with inorganic and organometallic complexes, figure 1, [2].

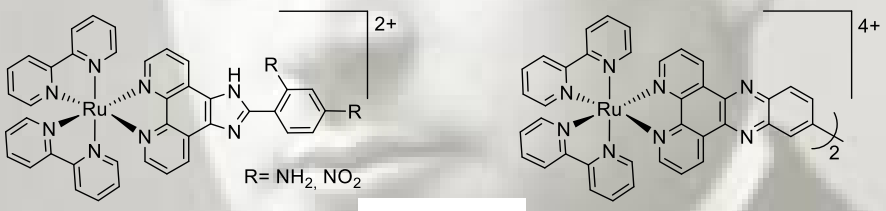

Fig. 1.

We present two representatives of ruthenium polypyridyl complexes whose moiety is $[Ru(bipy)_2(A\text{-}B)](CF_3SO_3)_2$ (A, B = N, P, As). Chelating ligands are necessary to give stability to final structure. Different ligands allow the modifications of the structure in order to improve their redox properties, solubility, etc. The cytotoxic activity of the compounds was also evaluated in human cancer cell lines A2780 (human ovarian carcinoma) and (human breast carcinoma). Ct-DNA interactions with the complexes by ultraviolet visible spectroscopy was studded because the DNA can be the target of ruthenium compounds [2] and electronic absorption spectroscopy is one of the most effective techniques for studying the binding mode of drug to DNA[3]. These studies were compared with the in *silico* results which were carry out with DNA sequence (CGCGAATTCGCG)2 obtained from the Protein Data Bank (PDB ID: 1BNA).

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Diet and hormones alter FNDC5 expression in different tissues and irisin serum levels

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Metabolic syndrome is characterized by a series of disorders closely related to each other's like insulin resistance, glucose intolerance and hyperlipidaemia [1]. Obesity is a very complex phenomenon in which plays very important roles peripheral tissues such as adipose tissue, liver, muscle and the neurohormonal and neurotransmitters dysregulation [2]. *FNDC5* gene encodes a secreted protein that is released from muscle cells during exercise, irisin. Initially, irisin was described as a myokine that induces white fat "browning" *in vivo* and *in vitro* [3], and later as adipokine [4]. Nowadays, is known like a new potential hormonal target for the treatment of obesity and type 2 diabetes. The aim of this study was to test if metabolic status regulates both central and peripheral *FNDC5* mRNA expression levels and serum irisin levels. Our study showed that *FNDC5* mRNA was expressed in high levels in muscle, brain and reproductive neuroendocrine axis. Blood irisin levels diminish after 48-h fasting and with leptin, insulin and alloxan treatments, but no changes were observed during long-term experiments with different diets. The increased *FNDC5* expression observed in different white adipose tissue depots could happen, or at least partially, in an attempt to compensate the decreased that occurs in the mass of those deposits during chronic caloric restriction, metformin and alloxan treatments. Hypothalamic *FNDC5* expression did not change for any tested diets suggesting that its regulation is not alimentation-dependent.

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UNDERSTANDING CHEMICAL REACTIONS USING QUANTUM CHEMICAL CALCULATIONS

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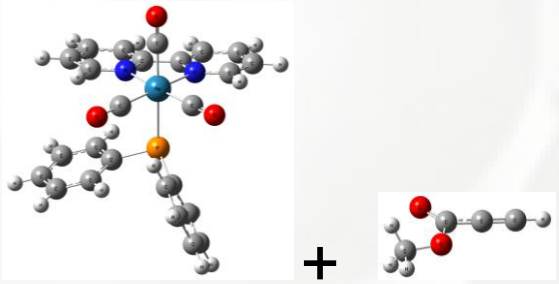
Theoretical and Computational Chemistry are relevant fields in the understanding of chemical problems. Particularly, Density Functional Theory (DFT) calculations are becoming a conventional tool to improve the knowledge of chemical reactions of great complexity. The steps involved, the nature of the intermediates, the kinetic barriers, and the thermodynamic stability of the products, are issues sometimes more accessible to computational chemistry than to experimental clarification. In this work a DFT study was undertaken in order to find all possible reaction routes of metal complexes with a terminal phosphanido ligand, such as [Re(CO)$_3$(bipy)(PR$_2$)], with an activated alkyne, considering different substituents bonded to the P atom. Experimental evidences [1] could be rationalized and a better understanding of the process at a molecular level could be gained.



[Re(CO)$_3$(bipy)(PPh$_2$)] HCCC(O)OMe

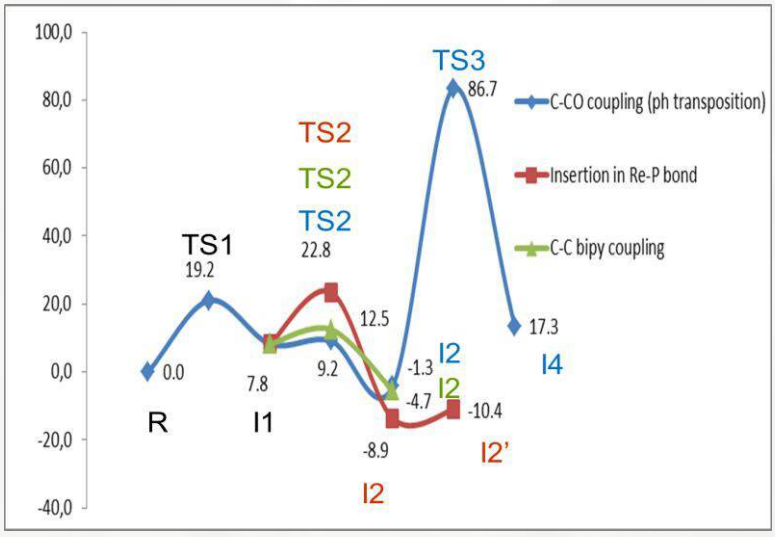


Fig.1 Energy profiles for the reaction of [Re(CO)$_3$(bipy)(PPh$_2$)] with HCCC(O)OMe

[1] Cuesta, L.; Hevia, E.; Morales, D.; Pérez, J.; Riera, V.; Rodríguez, E.; Miguel, D., *Chem. Commun*., 2005, 116-117.

Design of Ruthenium(II) compounds with promising biological properties

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Cis-$[Pt(NH_3)_2Cl_2]$ is considered as one of the most effective chemotherapeutic agents in clinical and nowadays the platinum-based chemotherapy is one of the most effective treatment for human cancers but its clinical application is limited by primary or acquired drug resistance, high toxicity and severe secondary effects[1]. The search for alternative compounds with promising anticancer activities has prompted chemists to develop alternative strategies to design, synthesize and evaluate the biological behaviour of many thousands of complexes derived from transition metals. One of these alternative elements is ruthenium, owing to its favourable properties, and some of its analogues such as NAMI-A and KP1019 are currently undergoing clinical trials. One of the main groups of ruthenium compounds which have been studied last years is that one derived from p-cymene and related ligands[2,3].

Here we present the synthesis of new compounds of Ru(II) with functionalized diphosphines via Michael addition reaction of nucleophiles to a C=C double bond (Figure 1). The complexes have been fully characterized and several biological tests have been undergoing.

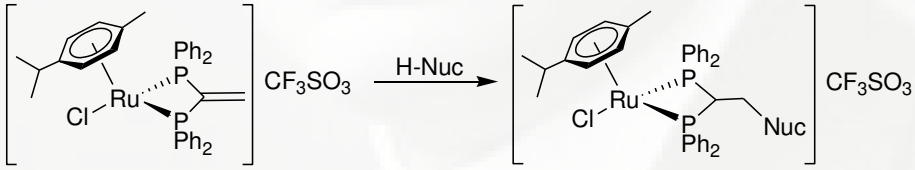

Figure 1: General Scheme of Michael Addition Reaction

[1] Rakesh Kumar Gupta, Amit Kumar, Rajendra Prasad Paitandi, Roop Shikha Singh, Sujay Mukhopadhyay, Shiv Prakash Verma, Parimal Dasb, Daya Shankar Pandey, Dalton Trans., 2016, **45,** 7163
[2] Alexey A. Nazarov, Christian G. Hartinger, Paul J. Dyson, Journal of Organometallic Chemistry 2014, **751**, 251
[3] Zenita Adhireksan, Gabriela E. Davey, Pablo Campomanes, Michael Groess, CatherineM.Clavel, Haojie Yu, Alexey A. Nazarov, Charmian Hui Fang Yeo, Wee Han Ang, Peter Dröge, Ursula Rothlisberger, Paul J. Dyson, Curt A. Davey; Nature Communications, 2014, **5,** 3462

Molecular magnetism in linear carborane polyradicals by means of local spins

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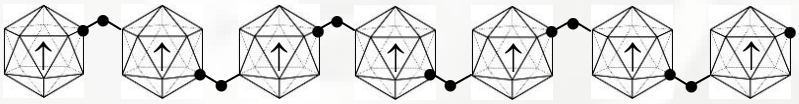
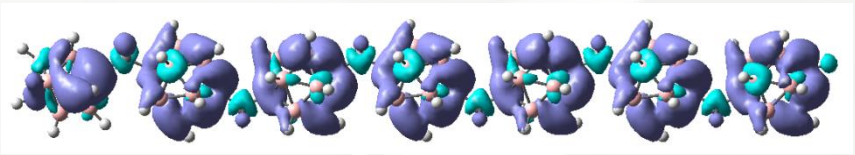
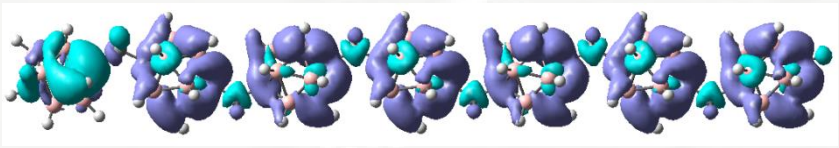
The electronic structure of simple polyhedral polyradicals composed of S=½ *closo*-carborane $CB_{11}H_{12}^{\bullet}$ structural units was recently reported [1,2]. Those works have been extended here in order to describe linear polyradical structures of these units connected by means of a $–CH_2–$ bridge. A mapping of the resulting spin states onto a Heisenberg spin Hamiltonian is proposed for these new linear chains, providing the evaluation of spin-exchange coupling constants and the analysis of their transferability.



(a)



(b)



(c)

(a) A chain of seven icosahedral carborane radicals $CB_{11}H_{12}^{\bullet}$ connected through $–CH_2–$ bridges with spin up (α basis function) for all cages. (b) The solution for the high-spin state (S = 7/2) with a plot of the spin density. (c) A constrained solution for the configuration | ↓↑↑↑↑↑↑ | with the corresponding spin density.

[1] J.M. Oliva, D.R. Alcoba, L. Lain, A. Torre, *Theor. Chem. Acc.* **132** (2013) 1329.

[2] J.M. Oliva, D.R. Alcoba, O.B. Oña, A. Torre, L. Lain, J. Michl, *Theor. Chem. Acc.* **134** (2015) 9.

Scanning Electron Microscopy for the identification of textile fibres

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The official methods for the quantitative chemical analysis of binary mixtures of textile fibres are an effective tool with which the market surveillance authorities can detect frauds. These methods are essential to ensure compliance in the European framework of the Regulation (EU) No 1007/2011 [1]. A proficiency testing scheme, with 29 laboratories from 15 countries, was provided by the Galician Laboratory of Consumer Products in order to guarantee the technical competence in this field. The samples were prepared and identified according ISO/TR 11827 [2]. One of the techniques applied for the identification were the scanning electron microscopy which was used to examine the longitudinal view and the cross section of the surface of the fibres under a scanning electron microscope using magnification (Fig 1). The images of the samples were compared with the images obtained by the reference materials in order to establish the appropriate correlations.

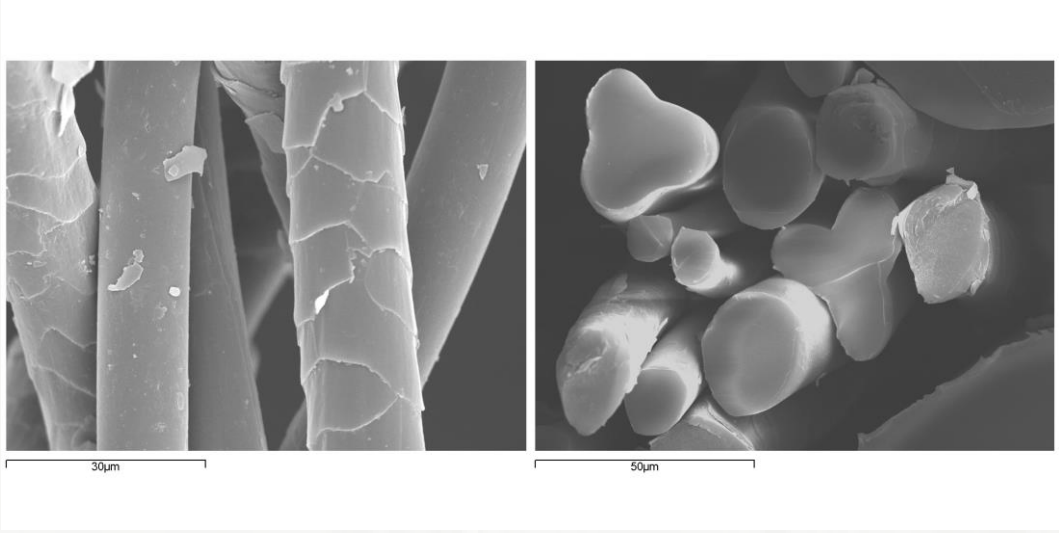

Fig.1 The longitudinal view and the cross section of the surface of some fibres

Acknowledges: To Catalina Sueiro López, Phd, for her technical support.

[1]. Regulation (EU) No 1007/2011 (2011) of the European Parliament and of the Council of 27 September 2011 on textile fibre names and related labelling and marking of the fibre composition of textile products and repealing Council Directive 73/44/EEC and Directives 96/73/EC and 2008/121/EC of the European Parliament and of the Council. Off J Eur Union L272:1–64
[2]. ISO/TR 11827 (2012) Textiles. Composition testing. Identification of fibres. International Organization for Standardization, Geneva, Switzerland

Biomedical Science Communication through Media from a Gender Perspective

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In our globalized world, the impact of the scientific knowledge, produced by several professionals, is constantly rising. Hence, biomedical research, integrated in health and welfare systems should constitute a driving force for economic and social development, creating wealth and consequently improving citizens quality of life and expectancy. Several studies indicate that STEM (Science, Technology, Engineering and Mathematics) professions present the highest growth prediction [1]. The current existent gap gender on these subjects, both at educative and RDI research levels, will have a tremendous impact in our economy if we don't develop strategies that don't underestimate the potential STEM talent female candidates [2]. Mass media represents a powerful toll to change social perception by disrupting and reshaping negative stereotypes about STEM women in science [3]. In "Women Scientists in Biomedicine: an endurance career" (Fig.1) we offer actions and tools to be integrated and distributed through mass media and new media (television, social networks, newspaper and radio), bridging the gap between biomedical science and society through female references of excellence. This project has allowed us to strengthen our commitment to biomedical female professionals in different phases of their scientific career, promoting their direct contact with young students, from different ages and educative stages, with special focus on girls. Their visions, experiences and background can enrich a global vision of biomedicine, stimulating students to broaden their perceptions on science and the scientific career, beyond their family, social and educative environments, encouraging them to enroll in STEM-based biomedical scientific professions, with a positive impact in welfare systems and thus patients health.

Fig.1 Women Scientists in Biomedicine.

[1] *Tertiary Education Participation,* Eurostat, 2013.
[2] *Women Scientists in Numbers: Statistics and indicators of gender (in)equality in the research career development.* MINECO, Madrid, 2013.
[3] P.G. Davies et al., *Personality and Social Psychology Bulletin*. **28** (2012) 1615-1628.

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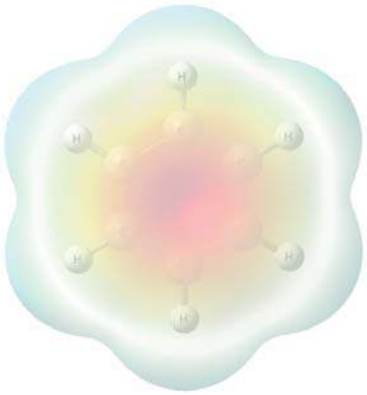
Cátedra Julio Palacios

I Simposio Internacional "Julio Palacios"

20 - 22 de julio de 2016 - Universidade da Coruña



Miércoles, 20 de Julio de 2016, 18:00 h

Conferencia pública (español)

"Julio Palacios y su tiempo"

Albino Arenas, UPM

Francisco González de Posada, UPM

21 - 22 de julio de 2016

I "Julio Palacios" International Symposium

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MARIA PAULA DIOGO, Universidade Nova de Lisboa (Portugal)

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