ZCAM and CECAM:

Present & Future

Zaragoza, 8-9 Junio, 2023


ZCAM
ZARAGOZA SCIENTIFIC CENTER FOR ADVANCED MODELING


cecam
Centre Européen de Calcul Atomique et Moléculaire


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f i
Instituto Universitario de Investigación
Biocomputación y Física
de Sistemas Complejos
Universidad Zaragoza


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1542


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ZCAM (Zaragoza Center for Advanced Modelling, es el nodo español del CECAM (Centre Européen de Calcul Atomique et Moléculaire).

Este encuentro ZCAM reúne a las diferentes comunidades que trabajan en el campo de la simulación computacional en España, con la presencia de Esther Martín Malagón, representante del Ministerio de Ciencia e Innovación (MCIN) en el Consejo de CECAM, y Andrea Cavalli, director del CECAM. Además, participan Ignacio Pagonabarraga, Michel Mareschal y Alberto Castro, anteriores directores de CECAM y ZCAM.

El objetivo de este encuentro es doble: promover el conocimiento, la participación y la organización de actividades en ZCAM y CECAM, y visibilizar la gran actividad científica realizada por investigadores españoles en este campo, mostrando la relevancia y vitalidad de las comunidades asociadas a CECAM en nuestro país.

A través de charlas invitadas que cubren diferentes áreas científicas asociadas a CECAM, presentaciones de los representantes institucionales, y una mesa redonda, se pretende recoger la visión de nuestra comunidad sobre la actividad futura de ZCAM y CECAM.

Comité organizador:

Rubén Pérez (Representante Científico del MCIN en el Consejo de CECAM, UAM)

Ignacio Pagonabarraga (director del CECAM 2017-2022, UB)

Verónica Ganduglia-Pirovano (ICP-CSIC)

Emilio Artacho (CIC nanoGUNE & Universidad de Cambridge)

Adrián Velázquez Campoy (director del ZCAM, UZ)

Day 1 – June 8th, 2023

Opening

- 15:00 - 15:10 – Adrián Velázquez Campoy (ZCAM & UZ)
- 15:10 - 15:30 – Welcome by the Organizers

Session I

Chair: Michel Mareschal

- 15:30 - 16:00 – Fernando Martín (UAM & IMDEA Nanociencia)
  Theoretical attosecond molecular dynamics: towards attochemistry

- 16:00 - 16:30 – Yamir Moreno (BIFI, UZ)
  Complexity, networks and systems thinking

- 16:30 - 17:00 – Modesto Orozco (IRB Barcelona)
  Nucleic acids: the molecules of Life and the drugs of the future. What can we learn from simulations

  17:00 - 17:30: Coffee Break

- 17:30 - 18:00 – Juan José García Ripoll (IFF-CSIC & QTEP)
  Quantum and quantum inspired opportunities for computation

- 18:00 - 18:30 – MCIN Representative

- 18:30 - 19:00 – CECAM Director

- 19:00 - 20:00 – Round Table

  21:30 – Event Dinner (Teatro Principal)

Day 2 – June 9th, 2023

Session II

Chair: Alberto Castro

- 9:00 - 9:30 – Javier Fernández Sanz (US)
  Computational modeling of heterogeneous catalysts

- 9:30 - 10:00 – Chantal Valeriani (UCM)
  A walk through active matter

- 10:00 - 10:30 – Carme Rovira (UB)
  How enzymes work. Insight from computer simulation

- 10:30 – 11:00 – Jorge Bravo (UAM)
  Harnessing AI in Materials Science: Current trends and a generative AI application

  11:00 - 11:30: Coffee Break

Session III

Chair: Pep Español

- 11:30 - 12:00 – Eva González Noya (IQFR-CSIC)
  Uncovering the assembly of colloids with directional bonds by computer simulation

- 12:00 – 12:30 – Luis Martín Moreno (INMA)
  Computational nanophotonics

- 12:30 - 13:00 – Remarks & Future Actions

Theoretical attosecond molecular dynamics: towards attochemistry

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The attosecond is the natural time scale of electronic motion in matter. Therefore, this time scale is key in chemistry. From water to DNA, all chemical reactions involve breaking and forming bonds, in which atomic nuclei are forced to live close to each other or to separate forever. But this is the consequence of the way electrons move. Thus, chemical reactivity results from the combined action of the "fast" electronic motion and the "slow" motion of atomic nuclei. Following the motion of the latter was possible by the end of the twentieth century with the help of femtosecond laser pulses. With the advent of attosecond light pulses at the dawn of the twenty first century, access to the attosecond time scale was finally at our reach. This was accomplished in 2010 [1] for the simplest molecule in nature, hydrogen, and, in 2014 [2], for phenylalanine amino acid. Since then, the field has grown exponentially, leading to a discipline called attochemistry [3]. All this progress would not have been possible without the guide of theoretical modelling [4]. Attochemistry is still at its infancy, but its long-term goal, achieving control of chemical processes by acting on electronic motion at its natural time scale does not seem to be a remote possibility anymore.

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Complexity, networks and systems thinking

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Complex Systems exhibit emergent system-wide properties that cannot be deduced from the behavior of their components, e.g., the whole is greater than the sum of its parts. Modern science has developed sets of tools that allow for tackling complex challenges where interdependencies play a key role. Here, we provide an overview of the above-mentioned techniques and show that the use of network and data sciences and mathematical modeling could provide novel insights and new perspectives to deal with scenarios in which a given system is subject to multiple -both in time and space- stresses. To illustrate the potentiality of the methodologies discussed, we discuss how network science and data-driven modeling have contributed to answering several key questions regarding the evolution of the COVID-19 pandemic.

Nucleic acids: the molecules of Life and the drugs of the future. What can we learn from simulations

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Nucleic acids are the central molecules of life. They not only store the genomic information, but they also modulate its expression and translation into proteins. In addition to these biological activities, nucleic acids display a variety of biotechnological and biomedical applications. Particularly, nucleic acids have emerged as new therapeutic tool and in fact RNA have become the most popular drug of the decade. What is the role of theoretical chemistry in this field? Can it help to understand the function of biological nucleic acids? Can it help to predict the activity of therapeutic nucleic acids?

Quantum and quantum inspired opportunities for computation

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[1]Institute of Fundamental Physics (IFF-CSIC) and CSIC Quantum Technologies Platform (QTEP)

In this talk I will briefly summarize the opportunities that arise for scientific computing in the dawn of quantum computing and quantum simulation. The talk will give an overview of quantum computers and quantum simulators as two hardware paradigms with different domains of applicability. It will also discuss how our understanding of these machines is opening new fronts in classical algorithms, the "quantum inspired" paradigm, an umbrella that encompasses new computational methods that originate in quantum mechanics and statistical and condensed matter physics. Finally, if time permits it, my talk will also briefly cover the European and national strategies for quantum technologies, from the Flagship projects to the integration of such technologies in communication (EuroQCI) and HPC (EuroQCS) infrastructures.

Computational modeling of heterogeneous catalysts

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Catalysis lies at the heart of chemical activity. In particular, more than 90% of current chemical processes rely on heterogeneous catalysis, with a huge economic impact across various key chemical industries such as oil refining, chemical synthesis, polymers preparation, energy production, environmental protection, etc.
As expected, optimization of catalytic processes and discovering of new, more efficient catalysts constitutes a major in research laboratories all over the world. Beyond the well-known trial-and-error traditional method of experimental laboratories, computational modeling of catalysts allows us to understand the way that a given catalyst works. This understanding provides a cost-effective alternative to improve and design new materials. In this talk, after a brief description of the catalytic phenomena, I will introduce the key aspects of computational methods to simulate different aspects and scales of surface reactions. The challenge of incorporating new strategies based on AI will also be addressed.

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A walk through active matter

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In the last 15 years, the Soft Matter community has paid an increasing attention in unravelling the Physics of Active Matter, a new and vibrant branch of Soft and Condensed Matter Physics.
Active matter systems are composed of non-equilibrium units that consume energy to perform directed motion. Examples of active particles at the mesoscopic scale are living, such as bacteria, or artificial, such as synthetic active colloids.
The theoretical framework describing these systems have shown tremendous success at finding universal phenomenology.
In my seminar I will present our contribution to the field of Active Matter, summarizing our work of the last ten years.

How enzymes work. Insight from computer simulation

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Enzymes are proteins that help speed up chemical reactions. Too much or too little of a certain enzyme can cause severe health problems, from rare lysosomal storage diseases to more prevalent ones such as cancer. One of the challenges of modern molecular biology and biotechnology is the design of specific drugs to block an enzyme that is dysregulated. Nevertheless, the molecular mechanisms of many enzymes remain unknown, which hampers the rational design of molecules that can interfere on their function. In this talk I will show how computer simulation is helping to understand how disease-relevant enzymes work and new efforts in this direction.

Harnessing AI in Materials Science: Current trends and a generative AI application

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This presentation will first spotlight current AI trends in Materials Science, drawing insights from the Spanish Network for AI in Condensed Matter Physics and Materials Science. In the second part of this talk, we will discuss our recent results on using Generative Adversarial Networks (GANs) in data-scarce spectral applications. The general aim of the talk will be to stimulate a discussion around how AI is shaping Materials Science and the potential and challenges it holds for the future.

Uncovering the assembly of colloids with directional bonds by computer simulation

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Experimental advances in the synthesis of colloids and nanoparticles with control over their shape and interactions [1,2] have opened an avenue for the design of new materials with desired functionalities. But to leverage the full potential of this approach it is necessary to decipher the relation between the particles' anisotropy and the ordered structures that they can form. Initially we addressed this problem by studying simple particle geometries, but the assembly behavior turned out to be fairly complex due to the usual appearance of competing structures [3-5]. Therefore, we reformulated the problem to that of designing the model system to obtain a given target structure, focusing on icosahedral quasicrystals (ICQ) which are materials that are ordered but lack periodicity in any direction of space. They were first discovered by Dan Shechtman in 1982 [6] and since then have been observed in many metallic alloys, but, so far, never in non-metallic or one-component systems [7]. We will show that they can be also obtained by using model particles with bonds that mimic the local environments in the target IQC [8]. We hypothesize that the designed models might be experimentally realizable in light of the impressive advances in the design of DNA origamis [9] and proteins [10].

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Computational nanophotonics

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Nanophotonics aims at the extreme concentration of electromagnetic modes for tailoring light-matter interactions and, through it, even modifying light-light and matter-matter interactions.
In the last few years, there has been a significant development in the theoretical capacity for computing the electromagnetic field distribution in complex environments from first principles.
In this talk, we will present some examples, highlighting the interconnection between the computations of optical properties of matter and those of electromagnetic fields.