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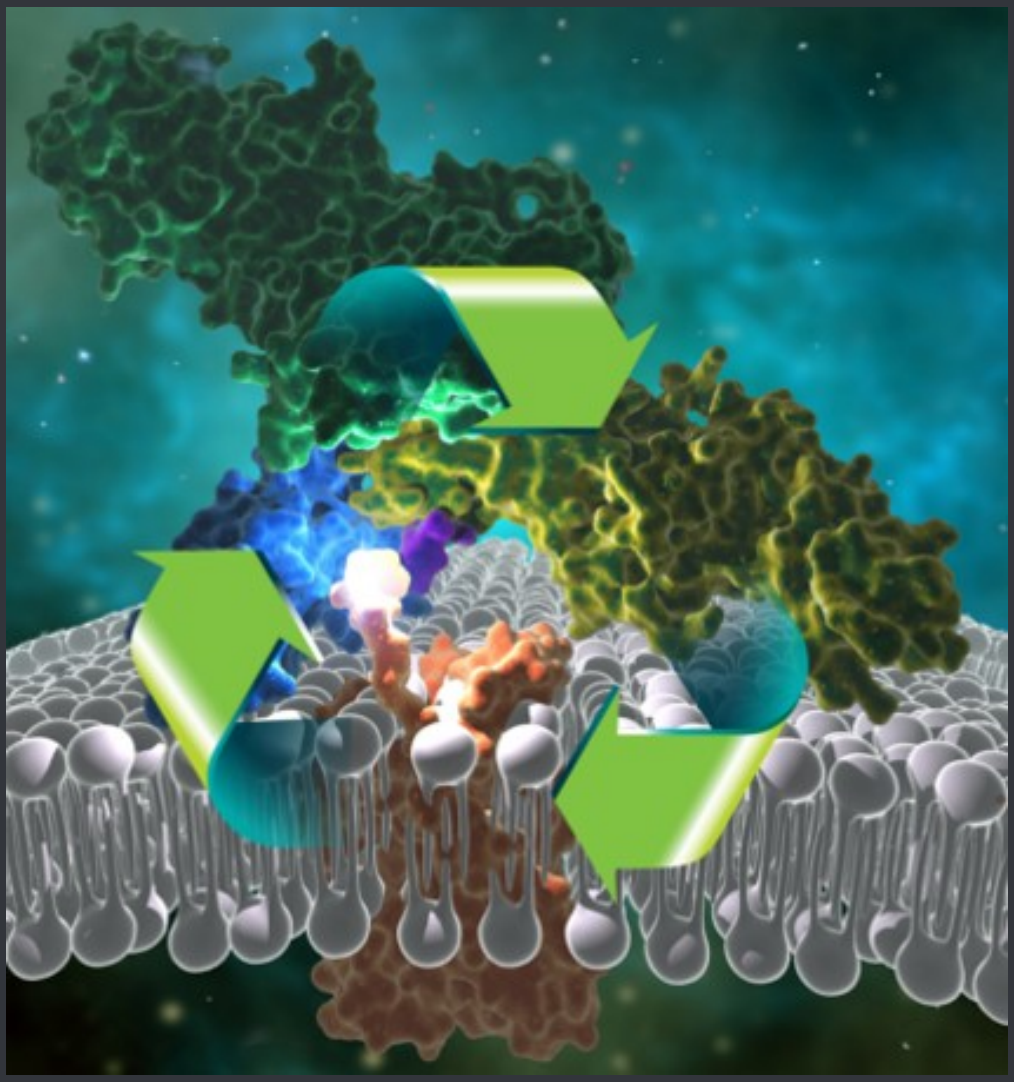

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Biofísica Magazine

EDITORIAL

The scientific societies today (particularly SBE):

Playground for interdisciplinarity and meeting point for science and society

Jesús Pérez-Gil
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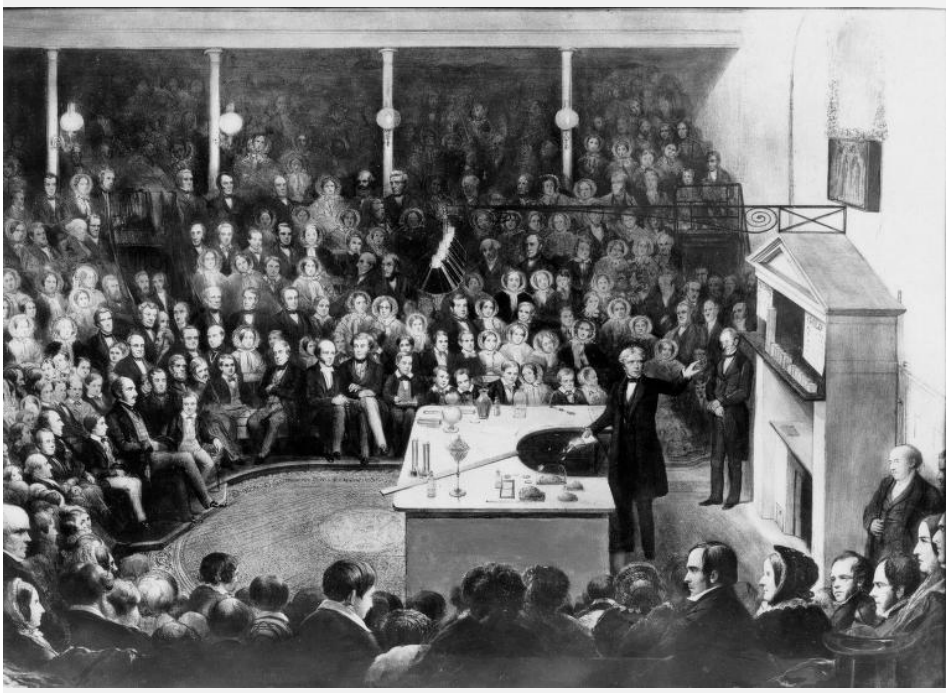
What is a *Scientific Society*? For many people this question may evoke classical pictures of a time when famous scientists defended their innovative studies in front of distinguished colleagues. Images like that represent historical sessions of the pioneering scientific societies that flourished since the XVII century. The Royal Society of London for Improving Natural Knowledge, simply known as *the Royal Society*, is a good example of them. Founded in 1660, it is considered the oldest scientific society in the UK and one of the oldest in Europe. In 2011, the Royal Society deservedly received the "Principe de Asturias" Prize on Communication and Humanities, being its current President the outstanding biophysicist Prof. Venkatraman Ramakhrisnan, who was awarded Nobel Prize in chemistry in 2009 for his seminal work on the structure of the ribosome.

Since their creation, the scientific societies have played a crucial role in spreading knowledge, both, regarding discussion and confrontation of novel theories and findings within the scientific community, and regarding the transfer of knowledge to the society in general. In the *old* years, there were few, if any, alternatives to consolidate and spread scientific research and knowledge. Thus, scientific societies started very early to create and support scientific journals, many of them still existing today. Soon, the societies also took the responsibility to organize periodic meetings and congresses, which continue being the basis for discussion and spreading of novel knowledge in all fields.

But, are these seminal roles of societies still important today?

Modern scientific communication and publishing has changed enormously, just during the latest



Michael Faraday delivering a Christmas lecture at the Royal Institution (1856).

few decades. The journals sponsored by societies (classical or new) nowadays coexist with a long list of new journals. Many of them are controlled by powerful and influential editorial groups, which operate outside the scientific societies and constitute the nucleus of a huge communication business. A lucrative business is also moving around the largest scientific congresses, which have now grown to reach a planetary scale. On top of that, a range of new digital technologies, with internet and the social networks at the front, allow a practically instantaneous worldwide diffusion of data and knowledge. In this context, one can wonder whether scientific societies still keep playing such an important role as in the past. What should be the goals of a modern scientific society, in particular a relatively small, national and specialized one like SBE?

> **We need the reference of a permanent and meditated meeting point for scientists, as well as for the encounter between scientists and the general public**

In my opinion, even in the current extraordinarily dynamic context, we need scientific societies in general, and the SBE in particular, to play a reflexive but still crucial role. In fact, perhaps more than ever, we need the reference of a permanent and meditated meeting point for scientists, as well as for the encounter between scientists and the general public. This meeting point must contribute to abolish the many barriers that the excessively compartmentalized structure of Spanish science imposes to modern research.

Let's apply the activity of SBE to promote an unlimited crosstalk between biologists, chemists, physicists, engineers... And let's do that with the goal of understanding fundamental problems which are important for people, concerning health, food, environment and general wellness. Science today has to be truly inter- and multi-disciplinary, or it will have no relevance. Although this is in principle an intrinsic property of the biophysics field, we know that the implementation of effective interdisciplinarity is a huge challenge. To start with, we need to support interdisciplinary education

> **Implementing effective interdisciplinarity is a huge challenge. We need to support interdisciplinary education and training policies**

and training policies, to aid our young people to progress in a less and less compartmentalized world. This transdisciplinary vocation and compromise must constitute a foundational and unalienable character of our SBE.

As important as being an interdisciplinary meeting point for research and education is promoting the encounter between science (and scientists) and the general public. We need forums to explain our science to the people and to facilitate the transfer of this knowledge for their benefit and progress. Only an efficient communication between research groups and the productive sector will allow the exploitation of innovative ideas and discoveries for the profit of the whole society. There should be no distinction between basic and applied science; there should only be good science, projected to its maximal extent. Let's show to our companies, industries, and hospitals the potential of high quality biophysical research. Scientific societies, like the SBE, have the responsibility of promoting the creation of novel and efficient channels of communication and transfer of knowledge. But we should also accept as a responsibility of SBE to explain everybody how the comprehension -both at qualitative and quantitative levels- of biological processes will allow us to live longer and better, and ultimately, to progress as a better society. This action on social communication can benefit today from extremely powerful tools, which a modern scientific society, such as SBE, has necessarily to embrace.

> **Scientific societies, like the SBE, have the responsibility of promoting novel and efficient channels of communication and transfer of knowledge**

New challenges, a long way to go and very important and unavoidable responsibilities. The Spanish Society of Biophysics is a young, modern and dynamic scientific society, which will know how to respond to the demands of this XXI century.

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Biofísica Magazine

BEYOND BIOPHYSICS

Translational Biophysics

A conversation with Antonio Ferrer-Montiel

José Villalaín Boullón
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From the bench to societal wealth... Bio-scientists do research because *we* really like and enjoy unveiling the secrets of how nature works. At the beginning, we love carrying out our research on the bench, and later and most of the time, leading and managing research programs. We all face plenty of obstacles when doing science; if we actually did not like it, scientists would have been *extinct* long ago. However, of course, as rare specimens, we love and enjoy our work on a daily basis. This is the central motivation to overcome the large number of difficulties that we encounter every day. If, on top of it, we add the possibility that our work can deliver perceptible benefits to society, the gratification is extraordinary.

Biophysics research, health, society, i.e., *translational biophysics*. Is it possible? The answer is simply and overwhelmingly, yes!

Antonio Ferrer-Montiel (Callosa d'en Sarrià, 1962) joined the University Miguel Hernández in 1997. He is full professor in Biochemistry and Molecular Biology and Director of the Institute of Molecular and Cellular Biology – IBMC. If we want to discuss about translational biophysics, he is definitely the right person to talk with. Why? He is the founding partner of several start-up biotech companies, such as Diverdrugs, Ilice Biotech, Prospera Biotech, AntalGenics and FastBase Solutions. He has 11 granted patents, 12 patents under evaluation, and 15 patents in exploitation. Apart from more than 100 publications, 25 reviews and 16 directed Ph.D. dissertations, he is involved in the scientific management of many founded projects from both institutional and industrial entities. He is also well known for his active compromise with different scientific societies and at the moment holds the presidency of the Biophysics Society of Spain – SBE.

Antonio has always shown an interest on understanding how membrane proteins work in terms of their underlying structure. First, he focused on membrane transporters and later he moved to the

field of ion channels. Since its incorporation to the IBMC, he has centred his research interests in the field of sensory neurobiology, aiming to uncover the role of ion channels in pain signalling. He uses this knowledge to identify novel therapeutic targets amenable for pharmacological modulation. This has prompted the development of a drug discovery platform that combines *in silico* screening and modelling, along with high throughput assays. As a result, several active molecules have been identified and one of them is currently under human clinical assays.

Professor Antonio Ferrer-Montiel.

Which is the road leading from basic to translational research? We will try to unravel this apparently tortuous process. Let us start at the very beginning: Biophysics; what is biophysics? Biophysics can be defined as the border of physics, biology and chemistry, encompassing everything connected between these fields; i.e. the quantitative understanding of how biological processes work at the molecular, cellular and system levels. Biophysics has evolved from the development and application of techniques, to monitor biological processes, to a discipline that aims to uncover the physical principles of biological function. This knowledge is essential for the correct development of biotechnology and biomedicine, thus having a high translational potential of its advances to our society.

> **Biophysical knowledge is essential for the correct development of biotechnology and biomedicine, thus having ahigh translational potential**

Antonio, knowing the relationship between *applied* and *basic* science, could you tell us which was your motivation to focus your research in science and, particularly, in biophysics?

> *The main motivation to become a scientist was my curiosity for understanding how nature works. Every time I look at nature's achievements, from physical to biological processes, I am astonished and have the necessity to understand them. I was attracted to biological processes because it amazed me how simple principles can be orchestrated to produce complex biological functions and, ultimately, life. I was captivated by the underlying mechanisms of cellular communication and, in particular, neuronal signalling. Truly amazing, yet, poorly understood processes are temperature and touch sensing, proprioception, nociception, cognition and learning. Thus, unveiling their molecular and physical principles is essential for intervening when they dysfunction (pain, cognitive disorders, etc). Undoubtedly, understanding how our brain works and encodes the information and its decision-making is a very exciting challenge.*

Very soon you realized the possibility of linking the basic research that you were pursuing with application in biotechnology and biomedicine. What moved you to include the word translational in your research?

> *It probably was the realization that knowledge has a tremendous value beyond its publication in a scientific journal. As Ikuro Nonaka says "In an economy where the only certainty is uncertainty, the one sure source of lasting competitive advantage is knowledge" As scientists, we like to disseminate our discoveries to the scientific community for its valuation and recognition. Notably, we also like to finish most of our papers with a significant statement (usually at the end of the discussion section) emphasizing the biotechnological and/or biomedical importance of our findings. In essence, virtually all scientists know that their results have potential important applications. I realized this and learned the ways to translate the generated knowledge into products and services for the benefit of our society.*

knowledge has a tremendous value beyond its publication in a scientific journal

It appears to me that there are scientific fields like biotechnology, chemistry, biomedicine, pharmacology, where translation is readily foreseen and heavily pursued, but it does not seem that clear for biophysics. What is translational biophysics?

> *In my opinion, biophysics is not different from other scientific disciplines. It generates knowledge on how biological processes work and how their dysfunction contributes to human diseases. In the past years, the progress of biophysics has been enormous, and with the development of more precise and sophisticated technology we are now examining biology at an unprecedented level, from single molecules to systems dynamics. We will witness that the biophysical knowledge obtained will have a huge impact on current societal challenges.*

Research is to not only discovering molecular structures and determining their function, but also to glimpse the different possibilities that can be obtained by changing those structures or even imagining new ones: *exploit the known, imagine the unknown and make it happen* . Such an innovative person like you, what is really in your mind: imagination...? Or, is it something that comes rolled along with research?

> *I believe that is a blend of everything. When thinking on a project I always like to look at the potential implications for society, and focus on understanding an specific problem, because with that knowledge comes the power to propose solutions and to transfer them for a societal benefit. Thus, what I hold in my mind is the necessity to make available and useful the scientific findings. When I do it, I feel that I am accomplishing something important. And, I should mention that exploiting the knowledge is not to reach an economical profit, but to make it accessible for those in our society that may need it.*

Often society is not able to discern the value of basic science. However, many products that people use in everyday life, not to mention everything related to health and wellness, are owed to it. What do you think that we, as scientists, have to say in order to show that applied research, what the society really sees, is due solely to basic research, what the society does not see?

> *We have to disseminate that there is good and bad science, and that good science gives rise to good applications for the benefit of society. I do not believe in the duality basic-applied science. It is clear that our society is only aware of the applications, and this is probably because scientists have not communicated in lay terms the scientific advances, their significance and their implications. Fortunately, this is rapidly changing with the implementation of out-reach activities sponsored by scientific societies, universities, research centres and researchers, as well as with the development and use of social networks. We are currently facing a revolution on science communication, and the society is understanding the importance of generating good scientific knowledge for increasing their wealth.*

There is good and bad science. Good science gives rise to good applications

We, scientists, may have a different perception of life , because, like it or not, we feel and see life in a different way. You, at the maturity of your life, after a long career in science but with many years still ahead, how much more could you ask in science?

> *In general, there are still plenty of societal challenges that need knowledge-based solutions, primarily, in medicine. Many diseases are yet without treatment or poorly treated; many current drugs have limited use because of adverse side effects. And with the increase in life-expectancy in our society, other maladies are becoming more prevalent. Thus, I see plenty of necessities for unveiling the molecular and cellular basis of diseases, identifying and validating biomarkers for diagnosis and prognosis, validating new therapeutic targets and developing better drugs, especially for chronic diseases. I believe that with the current technological developments the time is ripe for biophysics to take a lead in both, the generation and translation of knowledge.*

From the beginning to the end, from the biophysical bench to societal wealth... *through* translational biophysics. Throughout this conversation Antonio has shown us that it is possible nowadays to really perform translational research in biophysics; go from basic to applied research in a direct way. Perhaps many of us still do not realize the potential that biophysics has. So, we can only say one last word: Apply it!

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Biofísica Magazine

COOL BIOPHYSICS

Simulating Enzyme Catalysis

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Chemistry is about transformations between compounds as the result of forming and breaking bonds between their atoms. A detailed knowledge of these processes should open the door to one of the most desired goals in this field, which is the control of the rate constants that govern the time dependence of the concentrations of reactants and products. Changes in the concentration and preparation of the reactants, the nature of the solvents and external conditions (such as pressure and temperature) can be employed to speed up or slow down a chemical reaction. One of the major breakthroughs in the field of chemical kinetics was achieved when it was recognized that certain substances, *the catalysts*, were able to accelerate chemical reactions without being consumed during the process.

Living organisms use catalysts, known as enzymes, to accelerate chemical processes making them to take place in timescales compatible with life. The first observation of enzyme activity dates to the end of XVIII century. Amylase was the first enzyme to be isolated and urease was the first one to be identified as being a protein. Enzymes achieve rate enhancements as large as 1020 relative to the counterpart uncatalyzed reaction [1]. In addition, they present high efficiency, selectivity, few unwanted side products, and they usually work at aqueous mild conditions of pH, temperature or pressure, which converts them in very attractive catalysts for industrial purposes [2]. Nowadays we know that most of *biocatalysts* are proteins and the characteristics of these biomacromolecules, as discussed in this contribution, are responsible of their amazing catalytic properties. Many efforts have been devoted during the last years to understand the mechanism of action of these catalysts and to the practical implementation of this knowledge into the development of new biocatalysts.

The catalytic cycle of an enzyme involves at least three steps: substrate binding, chemical transformation and product release. The simplest kinetic scheme used to understand enzyme catalysis is that proposed by Michaelis and Menten, which involves the formation of a substrate-

catalyst complex previous to the actual chemical reaction:

$$E + S \rightleftarrows ES \longrightarrow P + E \quad (1)$$

We will focus here on the chemical step, showing how enzymatic chemical reactions can be analysed from a computational perspective and what have we learnt from these studies. We discuss theoretical approaches for the study of catalytic activity, consensus and discrepancies reached until now to describe the origin of this activity, and attempts to use all these findings in the development of new and more powerful catalysts.

Enzyme catalysis in Theoretical Chemistry

A complete understanding of chemical reactions requires an interpretation of the macroscopic observations (in this case the rate constant of the chemical step) from a microscopic perspective. The *Transition State Theory* (*TST*) is probably the most used theory to predict and interpret macroscopic rate constants from first principles [**3**]. TST establishes that the rate of a chemical transformation can be expressed as the probability to reach an activated conformation (or Transition State, TS) from the reactants (or Michaelis complex, ES in (1)) multiplied by the frequency needed for this complex to achieve the product state. The probability that reactants reach the activated conformation is given by the free energy difference with the TS, or activation free energy ($\Delta G^{\ddagger}$). The TST expression for the rate constant k_r of an unimolecular reaction (as the conversion from ES to P reflected in (1)) is then given by:

$$k_r = \frac{k_B T}{h} e^{-\frac{\Delta G^{\ddagger}}{RT}} \quad (2)$$

where the exponential factor accounts for the probability to achieve the TS and the preexponential term (where k_B is the Boltzmann constant, h is Planck's constant and T is temperature) is the universal frequency term. This theory is valid for many of the cases in which chemists are interested, except for those situations where thermal equilibrium is not reached or when light nuclei (hydrogen) are transferred. Nevertheless, even in this latter case, the TST expression can be corrected to account for those situations in which the light particle can tunnel through the energy barrier due to its non-classical nature.

The application of this expression to gas phase reactions of small molecules is quite straightforward. Chemical reactions are about electron reorganization which means that *quantum mechanics* (*QM*) is required. QM methods can then be used to obtain the energy of the molecules as a function of different coordinates that drive the system from the reactant state to the product state. For example, in a simple S_N2 reaction such, as $OH^- + CH_3Cl \rightarrow CH_3OH + Cl^-$ the distances associated to the bond to be broken ($C-Cl$) and the bond to be formed ($O-C$) can be used to obtain the potential energy of the system during the chemical transformation. Once the potential energy surface (PES) of the reaction is known (see **Figure 1a**) the free energies associated to the reactants and to the TS (and then the activation free energy) can be easily obtained using Statistical Thermodynamics under useful approximations, such as the harmonic behaviour of

molecular vibrations.

However, the picture becomes much more complicated when dealing with enzymatic reactions. First, the molecules under study are much larger, preventing the QM description of the full system. A realistic study of an enzymatic reaction must consider not only the substrate and the residues in the *active site*, but also the whole protein, possible cofactors, solvent molecules and ions. Typically, a realistic system designed to analyze an enzymatic reaction may easily contain thousands of atoms. Moreover, these studies must afford an additional problem: the large number of degrees of freedom of the system. The resulting PES (**Figure 1b**) is very rough, containing a hierarchy of valleys and sub-valleys of conformations that can be populated or not depending of the conditions in which the experiment is performed. The protein is not a rigid scaffold where the reaction takes place. Instead, the protein structure may suffer some changes during the reaction and the proper protein conformation must be chosen to obtain the right picture of the process. Thus the study of enzymatic reactions clearly requires the development of new methodologies, able to solve the problems associated to the size and conformational diversity of enzymes.

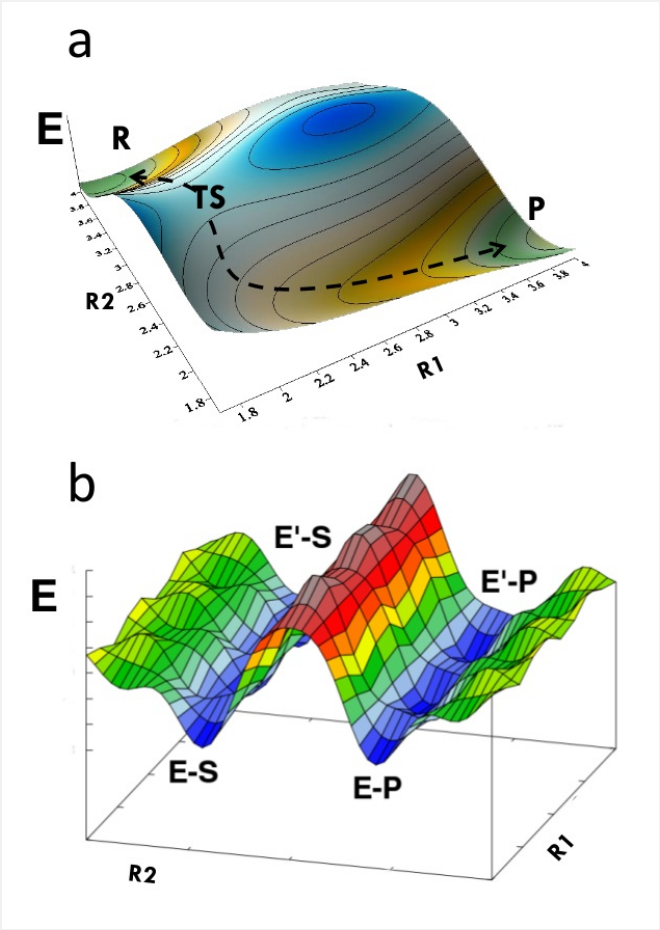

Figure 1. Potential Energy Surface corresponding to a chemical reaction. (a) *Small molecular system.* ***(b)*** *Enzyme. In large biomolecular systems there are myriads of possible stationary structures and the corresponding Potential Energy Surface is very rough. Simulations methods are needed to explore the relevant conformations of the system.*

New problems require new strategies

The 2013 Nobel Prize in Chemistry was awarded to Martin Karplus, Michael Levitt and Arieh Warshel for the development of multiscale models for complex chemical systems. Their pioneering work during the 70's [**4**,**5**] paved the way for modern computational strategies, allowing the study of chemical reactions in condensed media. The basic idea behind current methods is a partitioning of the whole system into two subsystems. The first one is described using QM methods and comprises all the atoms involved in the chemical reaction and then those atoms whose electrons must be explicitly described. The remaining part of the system is described using *Molecular Mechanics* (*MM*) interacting with the QM subsystem (**Figure 2a**). The resulting combination of methodologies is usually refereed to as *QM/MM hybrid methods* and takes advantage of both, the

reliability of quantum mechanics to describe bond breaking/forming processes and the efficiency of MM methods to evaluate the energy associated to conformational changes in the rest of the system.

QM/MM hybrid Hamiltonians provide the energy of the system. These methods can then be combined with Molecular Dynamics (MD) simulations in order to explore different configurations of the system. Different computational techniques, such as Umbrella Sampling, Metadynamics, Thermodynamic integration and others can then be employed to extract the variation of the free energy of the system when the reaction advances. These free energy profiles (**Figure 2b**) inform about the spontaneity of the process (the reaction free energy) and the rate (the activation free energy, see eq. (2)). This combination of methodologies, often refereed as QM/MM MD simulations, have opened the way to a vast number of studies of enzyme reactions which have been useful to elucidate a large number of reaction mechanisms and the role of specific enzyme residues in the catalysis [6]. This knowledge can then be used to rationalize, or even predict, the consequences of mutations on catalysis, which in turn can guide the design of new biocatalysts, as discussed below.

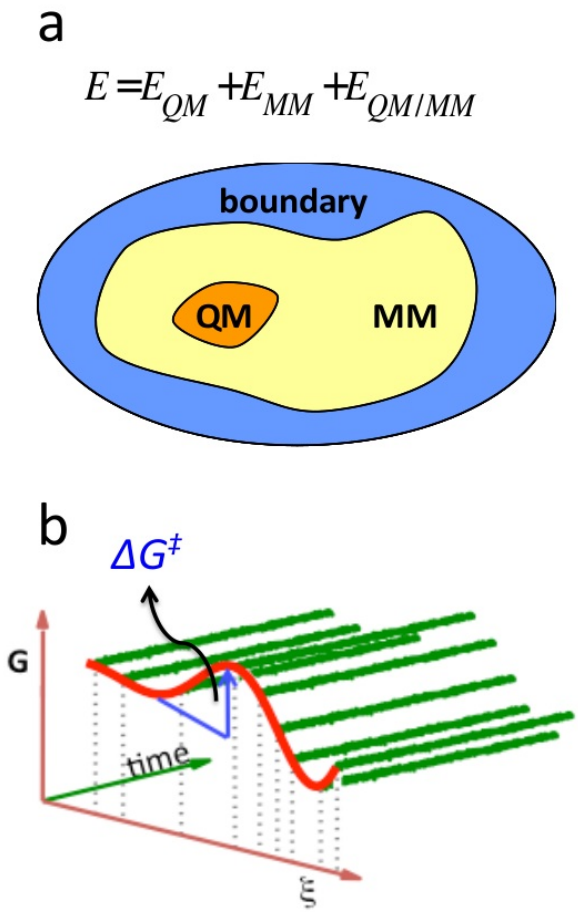

Figure 2. QM/MM methods for computational simulations of enzyme catalysis (a) *In hybrid QM/MM methods the total system is divided into a small region described at the QM level, where the chemical process of interest takes place, and the surroundings, described at the MM level. The total energy is the sum of the energy of the subsystems (E_{QM} and E_{MM}) and the interaction energy ($E_{QM/MM}$).* ***(b)*** *Molecular simulations can be carried out to obtain the free energy associate to changes along a particular coordinate. If this coordinate drives the system from reactants to products the activation free energy determines the rate of the process.*

Models to explain enzyme catalysis

Theoretical simulations of enzyme catalysis have been used to dissect the origin of the catalytic efficiency of enzymes. Nowadays, a growing consensus in the community is being reached around the seminal idea of Pauling [7], who assumed the complementarity between the enzyme's active site and the TS structure, originally expressed in terms of the *lock and key* analogy. The enzyme stabilizes more the TS than the Michaelis complex and thus the activation free energy appearing in eq. (2) would be lower than in the absence of the catalysts. Warshel and

co-workers [8,9] reformulated and quantified this hypothesis showing that the TS stabilization is basically due to the electrostatic environment provided by the active site of the enzyme. According to these authors, the active site displays an electrostatic environment prepared to accommodate the charge distribution of the reacting system at the TS. This provides a strong stabilization of the TS, relative to the reactants, without changing the enzymatic environment too much during the chemical transformation of the substrate. In contrast, in aqueous solution, water molecules can adapt to the reaction charge flow but, in most of the cases, an energy penalty, the reorganization energy, should be paid to rearrange the solvent molecules. These differences between the enzymatic and non-enzymatic reactions are qualitatively illustrated in **Figure 3**. The preorganization of the enzyme active site, which is a consequence of its tridimensional covalent structure, avoids the energy cost that must be paid in the uncatalyzed reaction to reaccommodate the solvent, lowering the activation free energy and increasing the rate of the process.

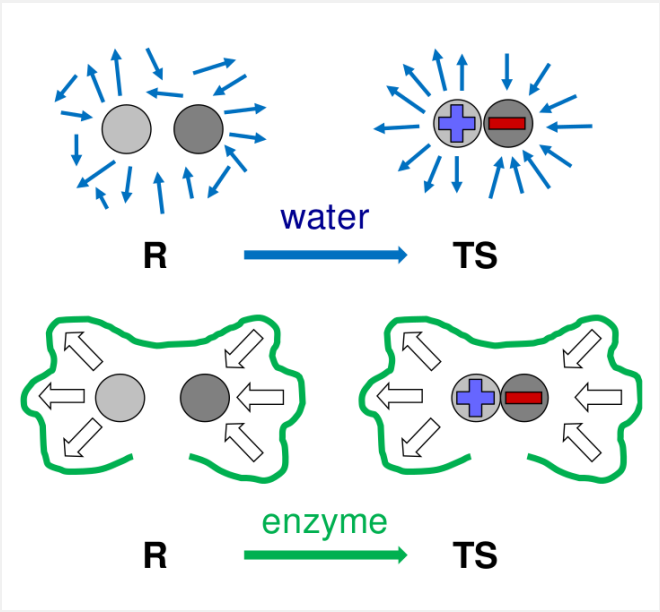

Figure 3. Reorganization around the substrate in the water solvent and in the active site of an enzyme. Top: *When a chemical reaction takes place in aqueous solution, water dipoles need to be reoriented to accommodate to the new charge distribution. The substrate is represented as spheres while water dipoles are represented by arrows.* ***Bottom:*** *The active site of an enzyme is preorganized to stabilize the charge distribution of the reaction Transition State, avoiding a free energy penalty and thus increasing the reaction rate. Arrows represent electrostatic interactions of the substrate with active site residues.*

Nevertheless, other theories have been invoked to explain the origin of the catalytic efficiency of enzymes. Some of the most popular proposals during previous years where those emphasizing the role of the enzyme in the formation of the Michaelis complex (ES in (1)). While the counterpart reaction in solution would require to approach and orient conveniently the reacting fragments, with a concomitant free energy cost, this rearrangement of the reacting fragments would occur in the enzyme already at the Michaelis complex and its free energy cost would be subsumed in the binding free energy. Thus, the key for the catalysis now focuses on the rearrangement of the substrate that takes place favourably in the enzyme active site and has an energetic cost in solution. In this sense Bruice et al. [10] introduced the concept of *Near Attack Conformations* (NAC), which are ground state conformers that closely resemble the TS. NACs would be as turnstiles through which the ground state must pass to reach the TS. According to this idea, the enzyme active site would decrease the activation free energy by increasing the probability of finding NAC-like structures.

Other explanations have been also invoked to explain enzyme catalysis. In the case of proton or hydride transfer reactions it has been suggested that enzymes could favour the transfer of these light particles by quantum tunnel behaviour, avoiding the necessity to overcome the energy barrier that is assumed in classical mechanics. Other authors have insisted in the role of coupling of protein vibrations with the chemical subsystem, in such a way that these vibrations could push the reacting system uphill along the energy barrier. However, when quantified with adequate simulations all these effects were shown to contribute very modestly, if any, to catalysis. [11–13]. The TS stabilization appears to be the major source for catalysis [14]. This idea can be then used to understand the role of protein mutations on the rate constant and to guide the design of new biocatalysts.

Nowadays there is a long list of enzymes that have been thoroughly investigated by means of flexible QM/MM techniques. These studies have been useful, not only to establish the corresponding reaction molecular mechanisms, but also, and probably more importantly, to investigate the principles of enzyme catalysis.

An illustrative example: the Catechol O-Methyl Transferase

The enzyme *catechol O-methyl transferase* (COMT) is an excellent prototypic system that has been the subject of extensive computational studies in several laboratories, including ours [13,15]. COMT, an enzyme that catalyzes the methyl transfer from S-adenosyl methionine (SAM) to catecholate, can be used to illustrate the role of the electrostatics interactions in catalysis. As shown in **Figure 4a**, the reaction consists in the transfer of a positively charged methyl cation from SAM to the negatively charged substrate (the catecholate anion). Thus, the reaction proceeds from charged reactants to neutral products. In aqueous solution this process is quite difficult because water molecules stabilize charged species by means of hydrogen bond and ion-dipole interactions. The solvation shell around the ions must be considerably distorted and the ions desolvate to allow the methyl transfer between them. This implies a free energy penalty to reach the TS from the fully solvated and separated reactants, increasing the activation free energy and thus reducing the rate of the reaction (**Figure 3**). In contrast, the active site of the enzyme is almost perfectly preorganized

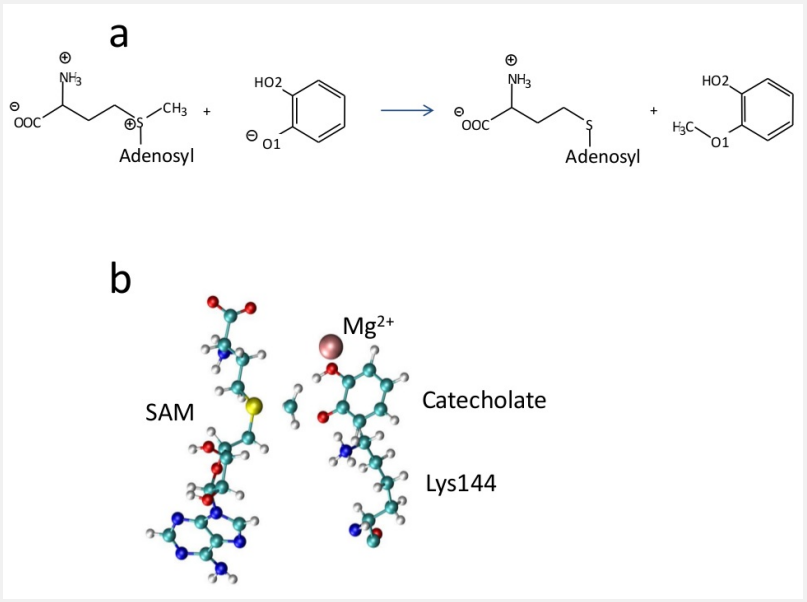

Figure 4. Reaction catalysed by Catechol O-Methyl Transferase. (a) *A methyl transfer from S-Adenosyl-Methionine to Catecholate.* ***(b)*** *Representation of the reaction Transition State in the enzyme with a* Mg^{2+} *ion bounded to the substrate.*

to stabilize the charge distribution of the TS, where the charge transfer between the two reacting fragments is considerably advanced because the methyl group is placed in between the donor sulphur atom and the acceptor oxygen atom (**Figure 4**).

The differences in the behaviour between the solvent and the enzyme can be illustrated following the free energy change associated to the reaction as a function of two coordinates: one measuring the advance of the reaction (the degree of methyl transfer from the donor to the acceptor atom) and the other one measuring the changes in the environment (which can be obtained from the electrostatic potential created by the enzyme on the donor and acceptor atoms). These two coordinates are qualitatively illustrated in **Figure 5a**. The free energy surfaces obtained as a function of these coordinates for the catalyzed and the uncatalyzed reactions are shown in **Figure 5b**. The most probable reaction paths from reactants (R) to products (P) crossing the TS are depicted as discontinuous lines on the free energy surfaces. The free energy surface corresponding to the reaction in aqueous solution shows that, in order to reach the reaction TS from the reactants, a large change must be done, not only in the reaction coordinate (i.e, the methyl group must be positioned between the donor and the acceptor atoms) but also in the environmental coordinate. Solvent molecules placed around the reacting fragment must be reordered to favour the methyl transfer. This large displacement along the environmental coordinate involves a large contribution to the activation free energy. However, the free energy surface corresponding to the same reaction in COMT clearly shows that in order to reach the reaction TS from the reactants (the Michaelis complex) a much smaller change is needed in the environmental coordinate. This illustrates the concept of *preorganization*: the electrostatic properties of the active site already in the Michaelis complex are close to that needed to reach the reaction TS, and thus a much smaller work must be done on the environment. This results in a smaller contribution to the activation free energy and thus in an increase in the observed rate constant with respect to the counterpart reaction in solution. The ultimate reason for this preorganization is found in the protein structure that results from the folding process and substrate binding. In this particular case, the presence of a conserved magnesium ion in the active site (**Figure 4a**) clearly contributes to create the adequate electrostatic environment for the reaction.

Perspectives in the field. Enzyme Design

Computational studies of enzymatic reactivity render a detailed knowledge on the source of the catalytic efficiency of natural enzymes that can be then used to guide the design of new generations of biocatalysts. The advantages of the use of biocatalysts in chemical and biochemical industrial processes are due not only to their ability to speed up chemical reactions by several orders of magnitude, but also with other inherent features of enzymes, such as their chemo-, regio- and stereoselectivity, and the ability to work under mild conditions of temperature and pressure. With the knowledge acquired from computational simulations, modified or even completely new enzymes can be designed and then prepared by means of protein engineering techniques. These new biocatalysts could then be used to catalyse the production of new valuable molecules or to substitute traditional industrial processes by cheaper, more efficient and more environmentally

friendly procedures.

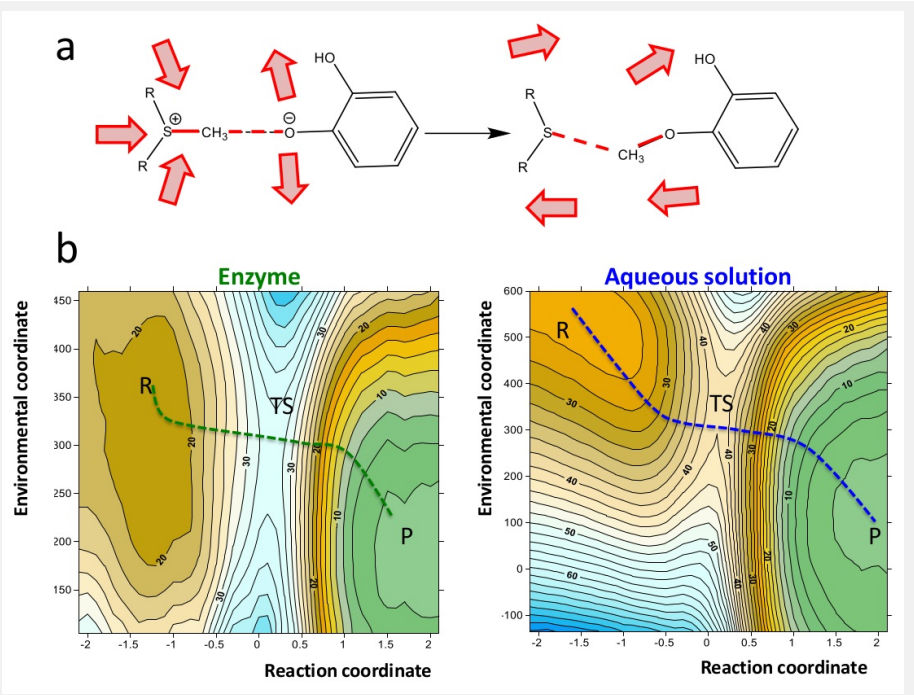

Figure 5. Two-dimensional coordinate description of the O-methyl transfer reaction. (a) *Catechol methylation in COMT and in aqueous solution can be followed using a reaction coordinate describing the degree of methyl transfer (changes in the solid and dashed red lines) and an environmental coordinate describing the changes in the surroundings (reorganization of red arrows).* ***(b)*** *The Free Energy Surfaces for the reaction in COMT and in aqueous solution show the different degree of preorganization in both environments. The reaction needs a larger change along the environmental coordinate in solution than in the enzyme.*

Different protein designs proposed to catalyse new chemical reactions during the past years can be classified, according to the strategy used in their development, into those based on directed evolution, rational design, or a combination of them known as semi-rational design [16]. Directed evolution refers to strategies inspired in natural evolution and consists in obtaining new proteins with new functions after some mutations or by recombination of protein fragments. The advantage of this strategy is that no structural information is needed *a priori* and that distant regions of the sequence space can be explored. Instead, rational design refers to the introduction of direct mutations of selected residues on specific positions of an already existing protein. These mutations, mostly in the active site or its close surroundings, are inspired in the analysis of data obtained from different sources, such as X-ray diffraction or, most recently, from computational simulations. When a protein without the desired catalytic properties is used as a scaffold to support an active site designed from scratch, the process is known as *de novo* design. This kind of rational design, pioneered by Mayo and co-workers [17], is based in the knowledge of the chemical reaction to be catalysed and, in particular, in its TS. In this case the first step for the design process is the construction of a minimalist active site to stabilize the TS charge distribution. This active site, often known as a *theozyme*, [18], is just a cluster of amino acids placed at adequate positions around the substrate to promote the reaction. At this stage, quantum mechanical methods are needed to properly describe the TS at the electronic level. Later, the minimal active site model is placed into an existing protein scaffold, selected from existing structural data bases. This step consists of several cycles of sequence design and protein structure optimization, followed by the ranking or scoring of the designed candidates.

The field has evolved from simply structural to more functional strategies, and from the design of just the primary coordination sphere of the active site to that of the secondary coordination sphere and beyond. Nevertheless, the amount of reactions catalyzed by computational based designed enzymes remains limited and, with some exceptions, the rate enhancements reached by these new biocatalysts is usually far from those of natural enzymes. The development of any of the different protein engineering strategies is hampered by the limitations of an incomplete understanding of enzyme structure–function relationships as well as by the inherent limitations of the employed experimental and computational techniques.

The design of new enzymes can be broadened by introducing metal ions in the active site. Metal-containing enzymes constitute a promising field due to the combination of the best features of homogeneous catalysis with enzyme catalysis; the broad catalytic scope and the high activity and selectivity under mild conditions, respectively. Nevertheless, since metal ions, or metal complexes, are involved in the process, the difficulties of designing this kind of biocatalysts dramatically increases [19].

From the computational point of view, different improvements have been incorporated during the past decade, such as considering the flexibility of the backbone of the protein scaffold, which was originally assumed rigid. As mentioned by Baker [20], *de novo* based design strategies can fail due to an imperfect theozyme, which does not represent the real TS of the reaction, a distortion of the designed active site into a given protein scaffold, or due to the effect of the long range electrostatic interactions and/or protein dynamics that can be incompatible with catalysis. Thus, further improvements on the *de novo* design of new enzymes must be based in a better localization and characterization of the TS by means of higher level computational methods.

The knowledge and simulation of long range electrostatic interactions can be used as a guide to the design of the new enzymes. Mutations far from the active site can be proposed to improve this kind of interactions. These methodologies can be extended to analyze the influence of mutations in steps like substrate binding or product release. This could improve the substrate affinity and/or the catalytic turnover, respectively. Consequently, the use of flexible molecular models treated by QM/MM multiscale methods, where the protein is introduced explicitly in the calculations, can be the bedrock of future successful studies. A proper sampling of the protein conformational landscape, performed by molecular dynamics simulations, could give also information related with the capability of a designed enzyme to catalyze a multistep-process. In this case, the active site of the enzyme has to be prepared not only to stabilize one TS but also to accommodate and stabilize the system for different steps. In addition, we should consider not only the TS stabilization but also the differential stabilization of the TS with respect to the reactants or Michalis complex [21].

The final goal in this field would be the design of a particular amino acid sequence that will fold into a particular structure with a desired function. This is still a chimera, but the incredibly rapid developments achieved in the last years allow predicting milestones truly breath-taking. Reaching this target will complete the round trip between theory and experiment, confirming theories and

computational tools developed in the field of the simulations of enzyme catalysis.

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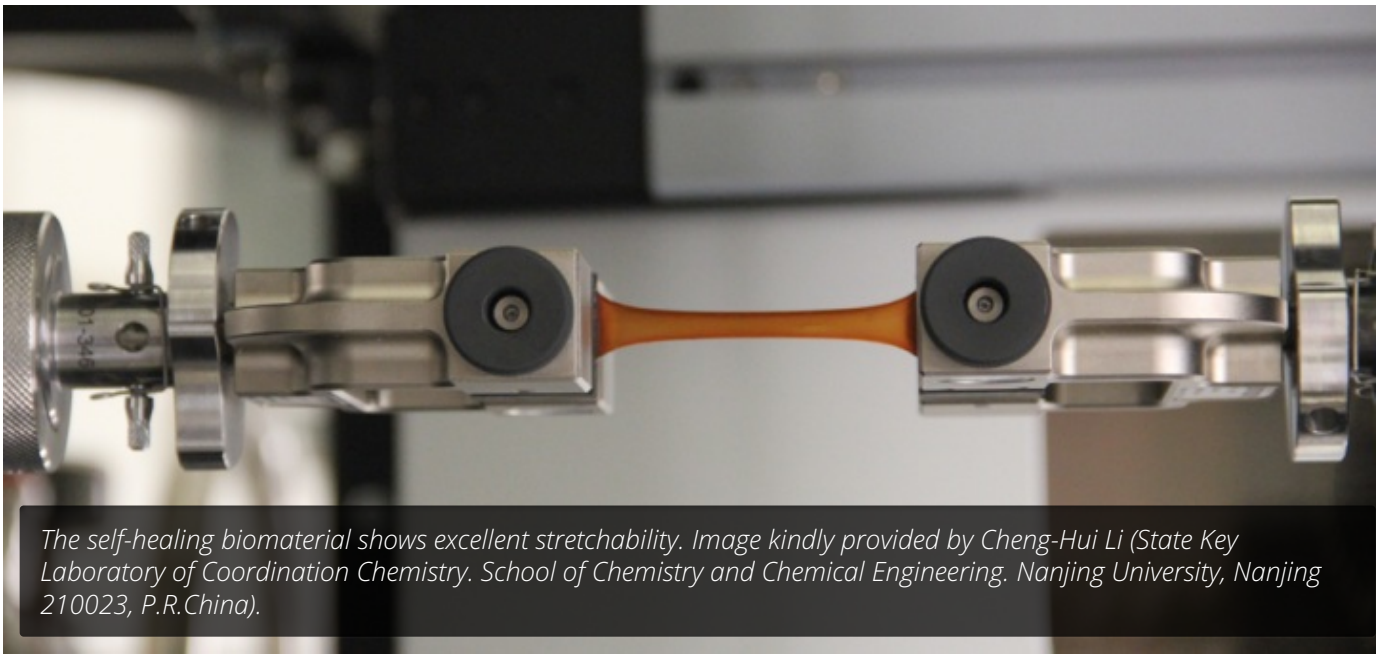
Biofísica Magazine

COMMENTARY – Stretch and heal: new elastomer self-heals when damaged



The self-healing biomaterial shows excellent stretchability. Image kindly provided by Cheng-Hui Li (State Key Laboratory of Coordination Chemistry. School of Chemistry and Chemical Engineering. Nanjing University, Nanjing 210023, P.R.China).

Carla Huerta-López, *CNIC, Madrid (Spain).*

Commentary to *A highly stretchable autonomous self-healing elastomer* (Li, et al. *Nat Chem*, **2016**, 8: 618).

Animal muscle is a natural biomaterial with remarkable properties: it is strong, elastic and able to undergo self-healing when damaged. Even though several polymers have been designed to mimic the behaviour of muscle, these characteristics have proven tough to mimic, and no material has been able to fulfil the existing gap in muscle tissue engineering. Therefore, it remains a challenge to synthesize materials that possess the properties of biological muscles.

A recently published paper by Cheng-Hui Li and co-workers describes a new stretchable elastomer, capable of self-healing without any energy input and independently of moisture conditions[1]. This material takes advantage of the versatility offered by metal-ligand interactions to achieve high strength and self-healing at room temperature. Working with Fe (III)-2,6-pyridinedicarboxamide coordination complexes, the authors were able to combine weak bond energies with low glass-

transition temperature. Thus, strong metal–ligand binding sites are adjacent to weak binding sites in the same ligand, where weak bonds can easily break dissipating energy, whilst the stronger interactions maintain the iron ions nearby allowing rapid weak bond re-formation.

Li *et al.* reported that the dynamic nature of the metal-ligand bonds, together with the easy breakage and reforming of the weak bonds, allows the unfolding and sliding of the polymer chains, rendering the stretchability of this elastomer to 45 times its original length (see **featured image** at the top of this text). These polymers are able to restore a high dielectric strength after being damaged. Furthermore, they show excellent self-healing ability even at low temperatures without any additive to promote healing. Taking it all together, the authors suggest that these elastomers are promising for tissue engineering applications, as smart and functional biomaterials.

It is undeniable that the design of new biomaterials is a growing field with potential impact in biomedicine, and this new elastomer could play an interesting role in this process. To this aim, there are some questions that still need to be addressed in order to improve the properties of this material. The natural following experiments would involve the study of its biocompatibility, both in cell culture and in animal models. Furthermore, related to some of the experimental results, it would be interesting to study the response of the material to the dielectric current of 11 kV, the one applied in the report, while it is still damaged. This could provide information for the use of the elastomer in tissue regeneration. It would also be useful to test if the material is able to respond to currents similar to the ones occurring in the muscles at physiological conditions (e.g -90 mV in cardiomyocites[2]).

Although this autonomous self-healing elastomer does not fully recapitulate yet the properties of animal muscle, it holds great promise for biomedical and tissue engineering, opening a door for future applications. Additional research will be essential to determine to what extent it may find room for use in the clinic.

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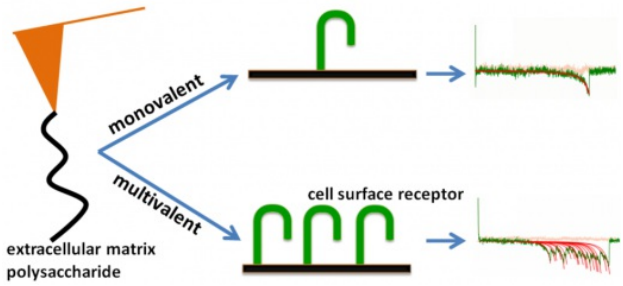
Biofísica Magazine

PAPERS OF THE MONTH BY SBE MEMBERS: SEPTEMBER - DECEMBER 2016

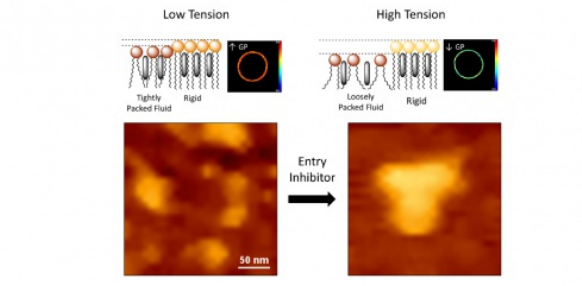


HIGHLIGHTS2016 / SEP. 2016

A single molecule assay to probe monovalent and multivalent bonds between hyaluronan and its key leukocyte receptor CD44 under force

Bano F, Banerji S, Howarth M, Jackson DG, Richter RP.

Sci Rep 2016 Sep.; 6: 34176.

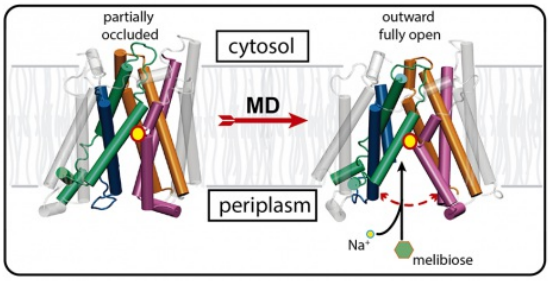


HIGHLIGHTS2016 / SEP. 2016

Functional organization of the HIV lipid envelope

Huarte N, Carravilla P, Cruz A, Lorizate M, Nieto-Garai JA, Kräusslich HG, Pérez-Gil J, Requejo-Isidro J, Nieva JL.

Sci Rep 2016 Sep.; 6: 34190.



HIGHLIGHTS2016 / SEP. 2016

Helical unwinding and side-chain unlocking unravel the outward open conformation of the melibiose transporter

Wang LY, Ravi VM, Leblanc G, Padrós E, Cladera J, Perálvarez-Marín A.

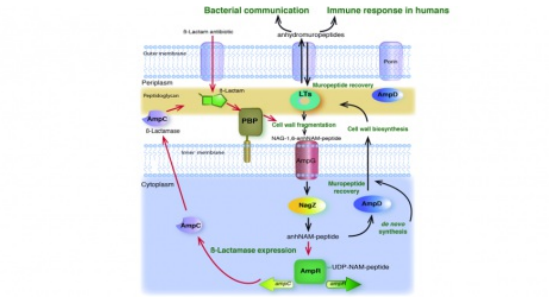
Sci Rep 2016 Sep.; 6: 33776.

HIGHLIGHTS2016 / SEP. 2016

Ceramide-Induced Lamellar Gel Phases in Fluid Cell Lipid Extracts

García-Arribas AB, Ahyayauch H, Sot J, López-González PL, Alonso A, Goñi FM.

Langmuir 2016 Sep.; 32: 9053.

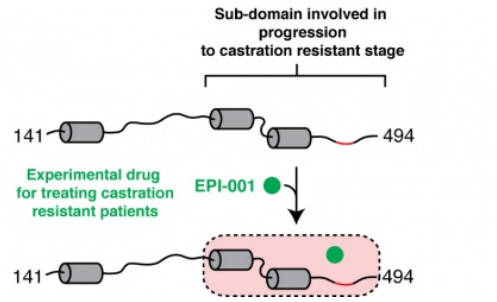


HIGHLIGHTS2016 / SEP. 2016

Renew or die: The molecular mechanisms of peptidoglycan recycling and antibiotic resistance in Gram-negative pathogens

Domínguez-Gil T, Molina R, Alcorlo M, Hermoso JA.

Drug Resist Updat 2016 Sep.; 28: 91.

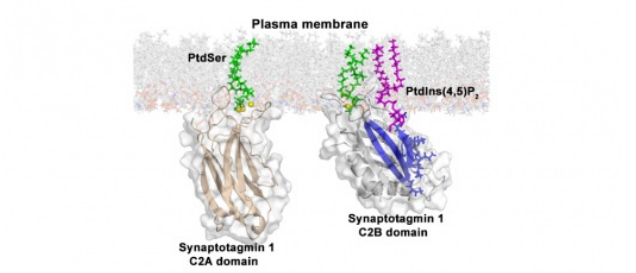


HIGHLIGHTS2016 / SEP. 2016

EPI-001, A Compound Active against Castration-Resistant Prostate Cancer, Targets Transactivation Unit 5 of the Androgen Receptor

De Mol E, Fenwick RB, Phang CT, Buzón V2, Szulc E, de la Fuente A, Escobedo A, García J, Bertoncini CW, Estébanez-Perpiñá E, McEwan IJ, Riera A, Salvatella X.

ACS Chem Biol 2016 Sep.; 11: 2499.

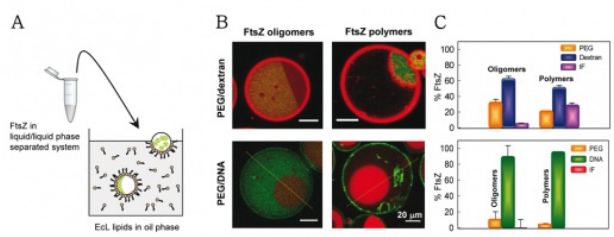


HIGHLIGHTS2016 / OCT. 2016

PtdInsP2 and PtdSer cooperate to trap synaptotagmin-1 to the plasma membrane in the presence of calcium

Ángel Pérez-Lara, Anusa Thapa, Sarah B Nyenhuis, David A Nyenhuis, Partho Halder, Michael Tietzel, Kai Tittmann, David S Cafiso, and Reinhard Jahn.

eLife 2016 Oct.; 5: e15886.

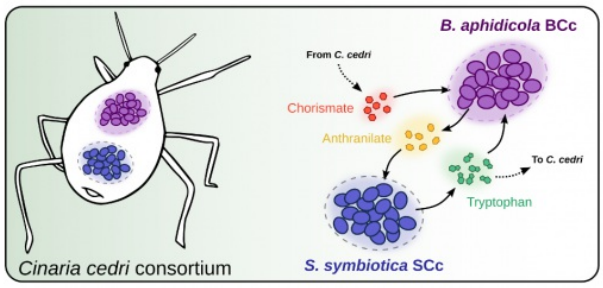


HIGHLIGHTS2016 / OCT. 2016

Microenvironments created by liquid-liquid phase transition control the dynamic distribution of bacterial division FtsZ protein

Monterroso B, Zorrilla S, Sobrinos-Sanguino M, Keating CD, Rivas G.

Sci Rep 2016 Oct.; 6: 35140.

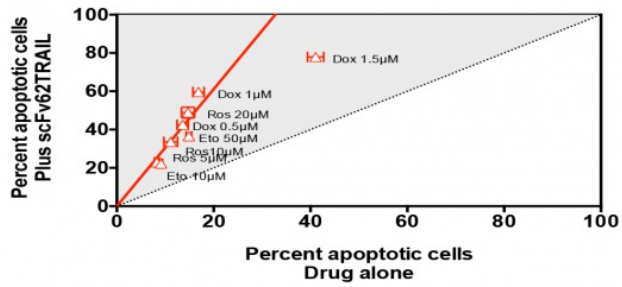


HIGHLIGHTS2016 / OCT. 2016

Metabolic Complementation in Bacterial Communities: Necessary Conditions and Optimality

Mori M, Ponce-de-León M, Peretó J, Montero F.

Front Microbiol 2016 Oct.; 7: 1553.

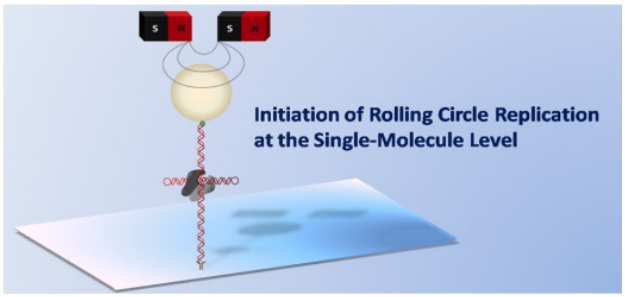


HIGHLIGHTS2016 / OCT. 2016

Guiding TRAIL to cancer cells through Kv10.1 potassium channel overcomes resistance to doxorubicin

Hartung F, Pardo LA.

Eur Biophys J 2016 Oct.; 45: 709.

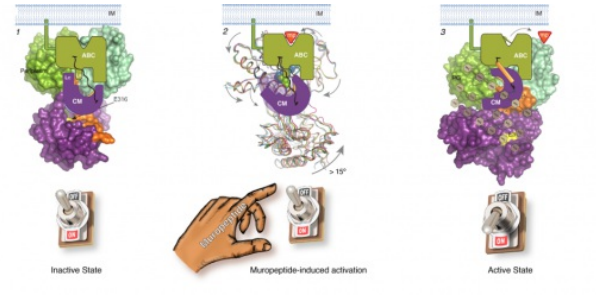


HIGHLIGHTS2016 / OCT. 2016

Force and twist dependence of RepC nicking activity on torsionally-constrained DNA molecules

Pastrana CL, Carrasco C, Akhtar P, Leuba SH, Khan SA, Moreno-Herrero F.

Nucleic Acids Res 2016 Oct.; 44: 8885.

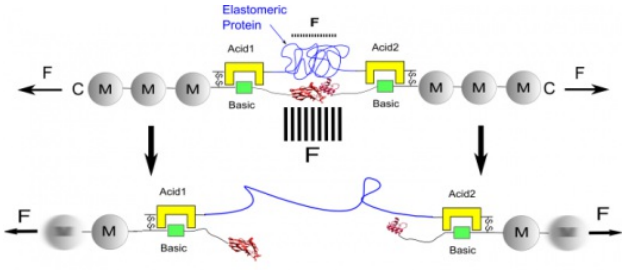


HIGHLIGHTS2016 / OCT. 2016

Activation by Allostery in Cell-Wall Remodeling by a Modular Membrane-Bound Lytic Transglycosylase from Pseudomonas aeruginosa

Domínguez-Gil T, Lee M, Acebrón-Avalos I, Mahasenan KV, Hesek D, Dik DA, Byun B, Lastochkin E, Fisher JF, Mobashery S, Hermoso JA.

Structure 2016 Oct.; 24: 1729.

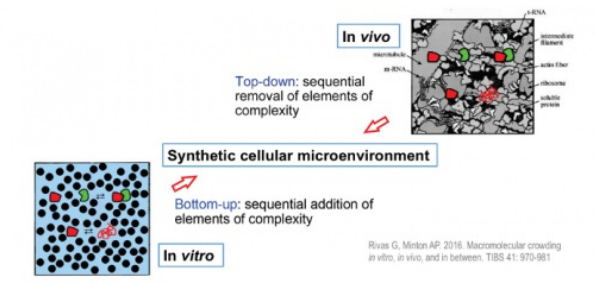


HIGHLIGHTS2016 / NOV. 2016

Direct Identification of Protein-Protein Interactions by Single-Molecule Force Spectroscopy

Vera AM, Carrión-Vázquez M.

Angew Chem 2016 Nov.; 55: 13970.

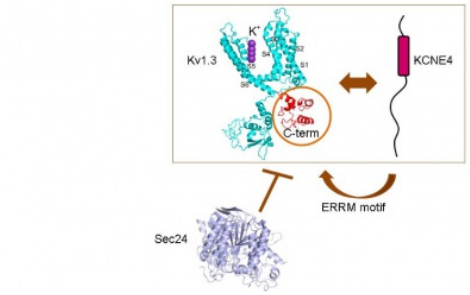


HIGHLIGHTS2016 / NOV. 2016

Macromolecular Crowding In Vitro, In Vivo, and In Between

Rivas G, Minton AP.

Trends Biochem Sci 2016 Nov.; 41: 970.

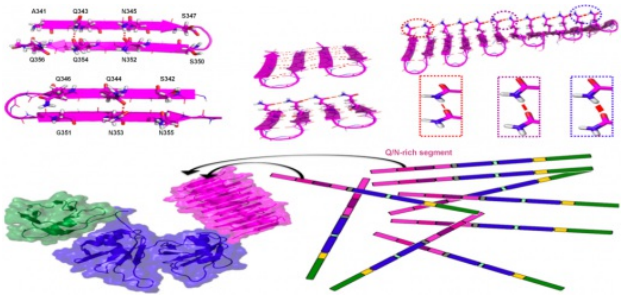


HIGHLIGHTS2016 / NOV. 2016

The C-terminal domain of Kv1.3 regulates functional interactions with the KCNE4 subunit

Solé L, Roig SR, Vallejo-Gracia A, Serrano-Albarrás A, Martínez-Mármol R, Tamkun MM, Felipe A.

J Cell Sci 2016 Nov.; 129: 4265.

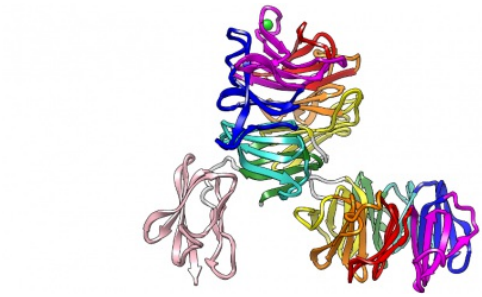


HIGHLIGHTS2016 / NOV. 2016

An Amyloid-Like Pathological Conformation of TDP-43 Is Stabilized by Hypercooperative Hydrogen Bonds

Mompeán M, Baralle M, Buratti E, Laurents DV.

Front Mol Neurosci 2016 Nov.; 9: 125.

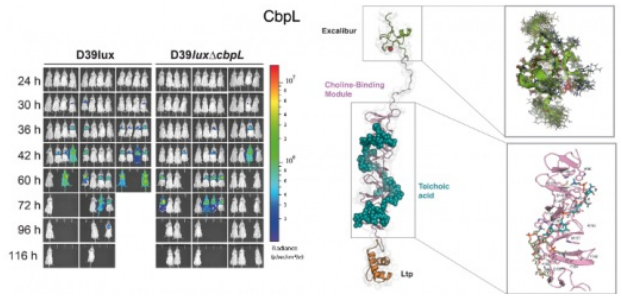


HIGHLIGHTS2016 / NOV. 2016

Structural and functional probing of PorZ, an essential bacterial surface component of the type-IX secretion system of human oral-microbiomic Porphyromonas gingivalis

Lasica AM, Goulas T, Mizgalska D, Zhou X, de Diego I, Ksiazek M, Madej M, Guo Y, Guevara T, Nowak M, Potempa B, Goel A, Sztukowska M, Prabhakar AT, Bzowska M, Widziolek M, Thøgersen IB, Enghild JJ, Simonian M, Kulczyk AW, Nguyen KA, Potempa J, Gomis-Rüth FX.

Sci Rep 2016 Nov.; 6: 37708.

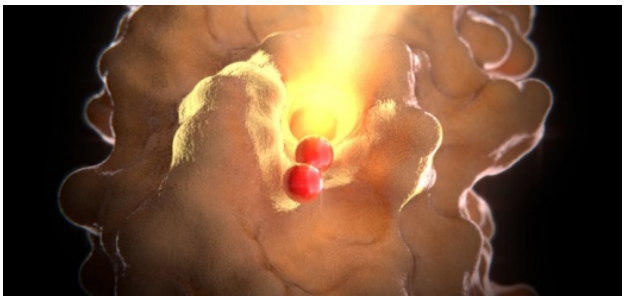


DEC. 2016 / HIGHLIGHTS2016

Modular Architecture and Unique Teichoic Acid Recognition Features of Choline-Binding Protein L (CbpL) Contributing to Pneumococcal Pathogenesis

Gutiérrez-Fernández J, Saleh M, Alcorlo M, Gómez-Mejía A, Pantoja-Uceda D, Treviño MA, Voß F, Abdullah MR, Galán-Bartual S, Seinen J, Sánchez-Murcia PA, Gago F, Bruix M, Hammerschmidt S, Hermoso JA.

Sci Rep 2016 Dec.; 6: 38094.

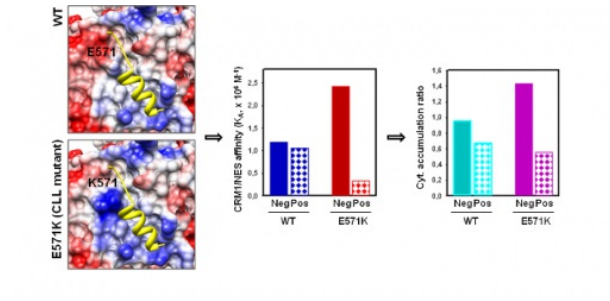


DEC. 2016 / HIGHLIGHTS2016

An oxygen-sensitive toxin-antitoxin system

Marimon O, Teixeira JM, Cordeiro TN, Soo VW, Wood TL, Mayzel M, Amata I, García J, Morera A, Gay M, Vilaseca M, Orekhov VY, Wood TK, Pons M.

Nat Commun 2016 Dec.; 7: 13634.

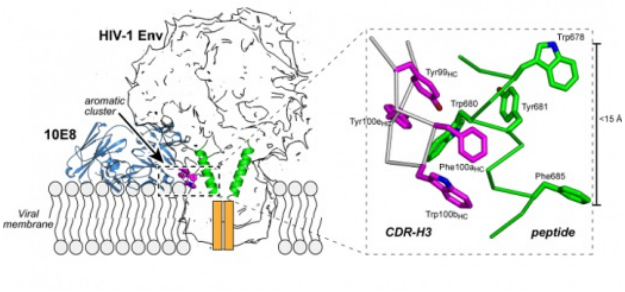


DEC. 2016 / HIGHLIGHTS2016

A cellular reporter to evaluate CRM1 nuclear export activity: functional analysis of the cancer-related mutant E571K

García-Santisteban I, Arregi I, Alonso-Mariño M, Urbaneja MA, Garcia-Vallejo JJ, Bañuelos S, Rodríguez JA.

Cell Mol Life Sci 2016 Dec.; 73: 4685.



DEC. 2016 / HIGHLIGHTS2016

Structural basis for broad neutralization of HIV-1 through the molecular recognition of 10E8 helical epitope at the membrane interface

Rujas E, Caaveiro JM, Partida-Hanon A, Gulzar N, Morante K, Apellániz B, García-Porras M, Bruix M, Tsumoto K, Scott JK, Jiménez MÁ, Nieva JL.

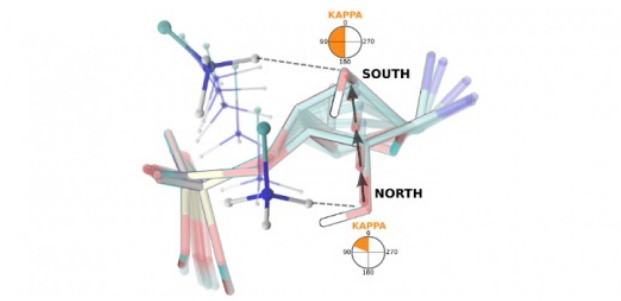
Sci Rep 2016 Dec.; 6: 38177.

DEC. 2016 / HIGHLIGHTS2016

Structural Mechanism for Cargo Recognition by the Retromer Complex

Lucas M, Gershlick DC, Vidaurrazaga A, Rojas AL, Bonifacino JS, Hierro A.

Cell 2016 Dec.; 167: 1623.

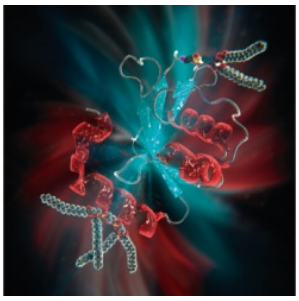


DEC. 2016 / HIGHLIGHTS2016

Small Details Matter: The 2′-Hydroxyl as a Conformational Switch in RNA

Darré L, Ivani I, Dans PD, Gómez H, Hospital A, Orozco M.

J Am Chem Soc 2016 Dec.; 138: 16355.



DEC. 2016 / HIGHLIGHTS2016

Human Atg8-cardiolipin interactions in mitophagy: Specific properties of LC3B, GABARAPL2 and GABARAP

Antón Z, Landajuela A, Hervás JH, Montes LR, Hernández-Tiedra S, Velasco G, Goñi FM, Alonso A.

Autophagy 2016 Dec.; 12: 2386.

Biofísica Magazine

AWARDS / NOMINATIONS / SBE PRIZES

SBE Prizes 2017 – Call for Nominations

The 2017 call for nominations to SBE Prizes is now open

The SBE offers yearly special awards to recognize the excellence in the field of Biophysics. These prizes are given in the following three categories:

XIV 'MANUEL RICO' – BRUKER PRIZE

DEADLINE JANUARY 30TH 2017.

> *Recognizes an outstanding Biophysics career, performed in Spain mainly during the last 10 years.*

Sponsored by

Bruker Española S.A..

Addressed to

Biophysicists working on Structure/Function of molecules who develope their main activity in Spain. **Preference** is given to members of the SBE .

Award

3000 € and a talk delivered by the awardee during a special session of the 16th SBE Congress (Sevilla June 6 – 8, 2017).

How to apply

E-mail a letter to José Miguel Mancheño, addressed to the President of the SBE (Dr. Antonio Ferrer Montiel), attaching a *Curriculum vitae* and a summary of your most relevant scientific achievements.

More information

See *here* the Complete Bases and instructions to apply.

Past winners of this prize

2016: F. Xavier Gomis-Rüth (Barcelona)
2015: Juan A. Hermoso (Madrid)
2014: Óscar Llorca (Madrid)
2013: José Manuel Sánchez Ruiz (Granada) and Félix Ritort (Barcelona)
2012: Antonio V. Ferrer Montiel (Elche-Alicante) and Marta Bruix (Madrid)
2011: Ignacio Fita (Barcelona)
2010: Modesto Orozco (Barcelona) and José Luis Rodríguez Arrondo (Bilbao)
2008: José García de la Torre (Murcia)
2006: Jesús Pérez Gil (Madrid)
2004: Javier Sancho (Zaragoza)
2002: José María Valpuesta (Madrid)
2000: Miquel Pons (Barcelona)
1998: Rafael Picorel (Zaragoza)

'E. PÉREZ PAYA' – SBE 40 PRIZE

DEADLINE JANUARY 30TH 2017.

> *Recognizes the trajectory of a Biophysicist with age under 40 with a special contribution to the progress of Biophysics in Spain.*

Sponsored by

BCN Peptid and Prima – Derm.

Addressed to

Biophysicists under 40 who develope their main activity in Spain. **Preference** is given to members of the SBE and to achievements from the last 10 years.

Award

1500 € and a talk delivered by the awardee during a special session of the 16th SBE Congress (Sevilla June 6 – 8, 2017).

How to apply

E-mail a letter to José Miguel Mancheño, addressed to the President of the SBE (Dr. Antonio Ferrer Montiel), attaching a *Curriculum vitae* and a summary of your most relevant scientific achievements.

More information

See *here* the Complete Bases and instructions to apply.

Past winners of this prize

2016: Raúl Pérez-Jiménez (San Sebastian)
2015: Irene Diaz Moreno (Sevilla)
2014: Fernando Moreno (Madrid)

Sponsored by SBE and Werfen-Izasa-Beckman-Coulter:
2013: Xavier Salvatella (Barcelona)
2012: José Manuel Gómez Vilar (Lejona-Vizcaya)
2011: Teresa Giráldez (La Laguna)
2010: Pau Bernardó (Barcelona)

ANTALGENICS – SBE 33 PRIZE

DEADLINE JANUARY 30TH 2017.

> *Recognizes a young Biophysicist with age under 33, who have contributed significantly to the developmen of Biophysics, in Spain and/or abroad.*

Sponsored by

AntalGenics.

Addressed to

Outstanding young Biophysicists under 33, independently of the country where their work has been done. **Preference** is given to members of the SBE.

Award

1000 € and a talk delivered by the awardee during a special session of the 16th SBE Congress (Sevilla June 6 – 8, 2017).

How to apply

E-mail a letter to José Miguel Mancheño, addressed to the President of the SBE (Dr. Antonio Ferrer Montiel), attaching a *Curriculum vitae* and a summary of your most relevant scientific achievements.

More information

See *here* the Complete Bases and instructions to apply.

Past winners of this prize

2016: Lorena Redondo-Morata (Marseille)
2015: Cecilia Artola (Madrid)
2014: Jorge Alegre Cebollada (Madrid)
2013: Anna Shnyrova (Bilbao)
2012: Sergi García Manyes (London)

Biofísica Magazine

SBE PRIZES

Imagin'Action 2017

SBE announces the second "IMAGIN'ACTION" image contest!

> *Launched on December 19th 2016 on the SBE social media and websites.*

Deadline and how to participate

Submit your images in electronic format by e-mail to community.manager@sbe.es before February 19th, 2017.

Extract of *Rules*

Download *here* the complete official rules

- Submitters must be registered members of SBE.
- Submissions are limited to max 3 images per contestant.
- Images may be obtained by any method, but must have a direct connection to biophysics.

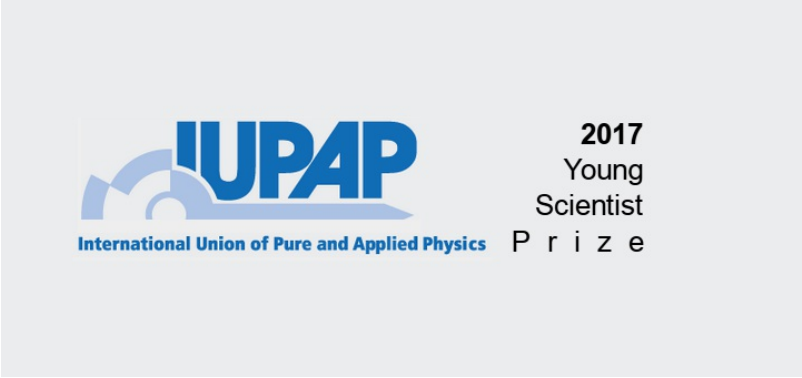
NOTE that the winner will be chosen 50% from public vote. Stay tunned with SBE social media: / !

- All images submitted must include a title and a short description (max. 50 words).
- The winner will be chosen among pre-selected images (max. 30) as a result of the following procedure: **a)** 50% out of Popular vote in SBE social media: / (between February 22nd and March12th, 2017. **b)** 50% out of punctuation given by a panel of judges.
- The prize, sponsored by Hamamatsu Spain, will consist on a free inscription to the 16th SBE Congress (Sevilla June 6th-8th 2017) plus € 250 to cover travel expenses.
- The winner and two other finalists will have their images displayed in the main hall at the location of the 16th SBE Congress.

Biofísica Magazine

AWARDS / NOMINATIONS

IUPAP C6 Young Scientist Prize: Call for Nominations



By The International Union of Pure and Applied Physics – IUPAP-Commission 6: Biological Physics

> *The IUPAP C6 Young Scientist Prize recognizes exceptional achievements of scientists in the field of Biological Physics at a relatively junior stage of their career.*

The recipient must be no more than eight years post PhD (excluding career interruptions) by the deadline of the competition and is expected to have demonstrated significant scientific achievements and displays exceptional promise for future achievements in Biological Physics.

The Prize

Three winners would be considered for the prize of 2017 (one prize per year 2015–2017). The individual prize will consist of 1,000 € award money, a medal, and a certificate. One prize cannot be shared between several candidates. The winners will have the opportunity to give an invited oral presentation at the 9 th IUPAP International Conference of Biological Physics ICBP2017, June 5–9, 2017 in Rio de Janeiro, Brazil, sponsored by the commission.

The prize selection committee will consist of all C6 commission members.

Applications

The deadline for nomination submission is March 8, 2017. Self-nominations are not permitted, but a candidate could ask a mentor or colleague to provide a nomination. The nomination package should be bundled into a single pdf file called Surname_ysm.pdf, where Surname is the candidate's name, and should include:

1. A brief statement on the achievement for which the nominee is to be recognized.
2. Curriculum vitae including all publications.

Nominations should be send by e-mail to the chair of the award committee,Helmut Grubmüller, Vice-Chair of C6, together with cc's to Aihua Xie, Chair of C6, and Rita Maria Cunha de Almeida, Secretary of C6.

IUPAP welcomes applications from outstanding women and other underrepresented groups.

More information

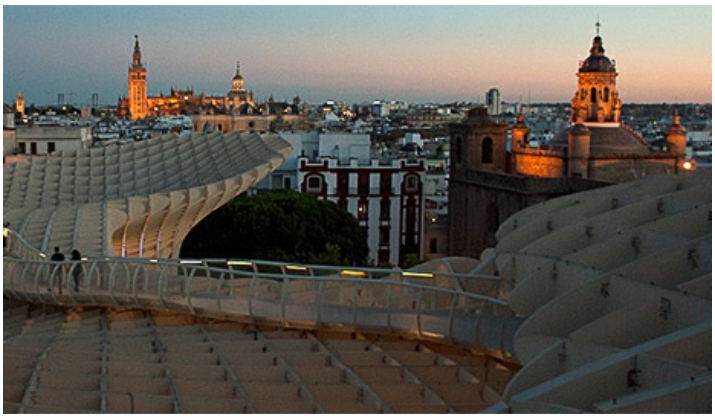
Please, visit the IUPAP Website.

Biofísica Magazine

16th SBE Congress

Annual Meeting of the Spanish Biophysical Society. **June 6 – 8, 2017**, Sevilla (Spain).

Presentation



On behalf of the Organizing Committee, it is a great honor to invite you to attend the 16th Congress of the Spanish Biophysical Society – SBE, which will be held at cicCartuja on 6-8 June 2017.

The scientific program is comprised of Plenary Lectures, together with Parallel Symposia focused on the most challenging topics in Biophysics. Symposia will include not only invited talks addressed by well-recognized scientists but also short communications selected from submitted abstracts. In this regard, an effort to give preference to young researchers will be made.

The program leaves enough time for fruitful and lively discussions, especially during Poster Sessions. The singularity of the 16th Congress of SBE is the activity Biophysics in the City, which aims to bring Biophysics closer to society.

As per usual, reduced registration fees will be charged to participants who are SBE members.

Moreover, a number of grants funded by SBE to encourage young researchers' participation are available.

We will endeavor for the 16th Congress of SBE network meeting to have a high rate of participation, since throughout the years our Congress became the perfect forum for scientists doing research in Biophysics.

Looking forward to welcoming you to Seville.

Best regards,

Irene Díaz-Moreno, Chair of the Organizing Committee

Deadlines

- Nominations for SBE Prizes: January 30th 2017.
- Imagin'Action image contest: February 19th 2017.
- Application for Bursaries: February 19th 2017.
- Early Registration (low fee): March 19th 2017.
- Late Registration and Abstract Submission: April 15th 2017.

More information

Please, visit the Congress Web Site.

Biofísica Magazine

CONFERENCE REPORTS / EVENTS / MEETINGS / NEWS

SBE Members Participate in III LaFeBS Meeting

BY BIOFISICA · PUBLISHED 29/11/2016 · UPDATED 26/01/2017

Coorganized by the biophysical societies of Argentina, Brazil, Spain, Portugal and Uruguay

A delegation of the SBE, composed by the former presidents Alicia Alonso and Juan Carmelo Gómez-Fernández, and by Carlo Manzo, attended the III Latin American Federation of Biophysical Societies (III LAFeBS) – IX IberoAmerican Congress of Biophysics – XLV Reunion Anual SAB 2016 in Sant Miguel de Tucuman, Argentina on November 23-25 2016.

The Argentinian Biophysical Society has been organizing this meeting since its foundation, 45 years ago, with the aim of congregating scientist that conduct original research and to thus promote the development of Biophysics. This year, to commemorate the two-hundredth anniversary of the Declaration of Independence in Tucuman, the LaFeBS Bicentennial meeting has been organized together with the biophysical Societies of Brazil, Spain, Portugal and Uruguay. The opening symposium has been dedicated to the memory of Gregorio Weber, for his remarkable scientific career and outstanding contributions to the field of Biophysics.

The congress hosted more than 250 scientists from all the organizing countries. The 3-day program included 7 plenary sessions and 10 topical symposia, embracing all the areas of biophysics. Lively

poster sessions including more than 70 participants animated the lunch breaks. The welcome cocktail was held in the monumental White Room of the baroque Government House of San Miguel de Tucuman in the presence of local authorities.

Biofísica Magazine

CATEGORY: EVENTS

Upcoming Meetings, Courses and Workshops

EVENTS / WORKSHOPS 24/10/2016

1st Biology for Physics Conference: Is there new Physics in Living Matter?

DPL Workshop January 15 – 18, 2017, Barcelona (Spain). Deadlines December 11th, 2016 (extended). Abstract submission January 8th, 2016. Registration The workshop aims to bring...

EVENTS / WORKSHOPS 14/11/2016

Advances in Single-Molecule Research for Biology & Nanoscience

XIX. Annual Linz Winter Workshop February 3 – 6, 2017, Linz (Austria). Deadlines October 15th, 2016. Early registration December 1st, 2016. Registration and abstract submission...

EVENTS / MEETINGS 14/09/2016

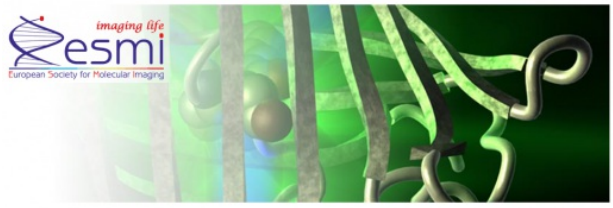
61st BPS Annual Meeting

61st Biophysical Society Annual Meeting. February 11 – 15, 2017, New Orleans, Louisiana (USA). Deadlines January 9, 2017. End of early bird registration October 3,...

COURSES / EVENTS 07/06/2016

Winter School: Biology at different scales

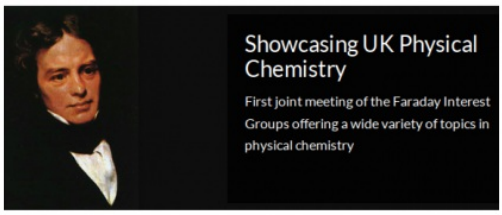
Winter School in Les Houches, France March 13 – 25 2017 The school will focus on the interplay between physics and biology to understand biological...



EVENTS / MEETINGS 24/10/2016

12th European Molecular Imaging Meeting – EMIM

April 5 – 7, 2017, Cologne (Germany). Deadlines January 11st, 2017. Abstract submission February 14th, 2017. Early registration What you can expect: It's all about...



EVENTS / MEETINGS 26/01/2017

Faraday Joint Interest Group Conference 2017

Joint meeting of RSC Faraday interest groups, including Biophysical Chemistry April 11 – 13, 2017, Warwick (UK). Deadlines March 14th, 2017. Registration for those wishing...

AWARDS / EVENTS / MEETINGS / NEWS / NOMINATIONS / SBE PRIZES
07/11/2016

16th SBE Congress

Annual Meeting of the Spanish Biophysical Society. June 6 – 8, 2017, Sevilla (Spain). Presentation On behalf of the Organizing Committee, it is a great...

EVENTS / MEETINGS 19/10/2016

Conformational Ensembles from Experimental Data and Computer Simulations

August 25 – 29, 2017, Berlin (Germany). Deadlines May 1st, 2017. Early registration This meeting aims to bring together scientists from across disciplines to advance...

EVENTS / MEETINGS 07/11/2016

42nd FEBS Congress

September 10 – 14, 2017, Jerusalem (Israel). Deadlines June 1st, 2017. Early registration The FEBS Congress aims to provide an outstanding international forum in the...

EVENTS / MEETINGS 19/10/2016

IUBMB Focused Meeting on Molecular Aspects of Aging and Longevity

October 16 – 19, 2017, Athens (Greece). Deadlines May 1st, 2017. Abstract submission May 1st, 2017. Fellowships June 1st, 2017. Early registration Aging is an...

Biofísica Magazine

CATEGORY: JOBS

Positions in Biophysics

JOBS / POSTDOC 18/01/2017

Postdoc position on cellular membrane biology and biotechnology

The Endocytic Trafficking and Intracellular Delivery team in the the Chemical Biology Department of the Institut Curie in Paris (France) is recruiting a post-doctoral researcher...

JOBS / POSTDOC 17/01/2017

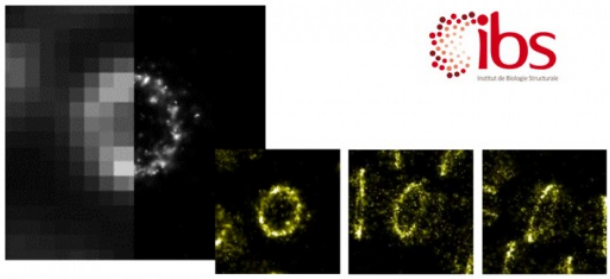
Posdoctoral Position in METABOLOMICS

Funded by MINECO Grant RTC-2016-5239-2 Topic: Metabolomics for the improvement of organoleptic quality in organic agriculture. The work will be performed at the University of...

JOBS / POSTDOC 17/01/2017

Postdoctoral Positions in Biomolecular Simulations

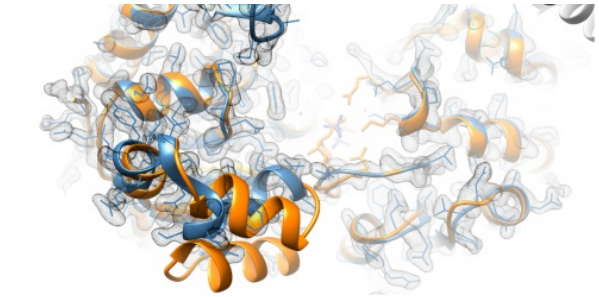
Postdoctoral positions funded by the ANR @RAction program within the project Multiscale Modeling of Biomolecular, to work at the Centre de Biochimie Structurale (IBS) Montpellier...



JOBS / POSTDOC 17/01/2017

3-year post-doctoral position: Super-resolution imaging of bacterial division

Applications are opened for a postdoctoral position at the Pneumococcus group – Institut de Biologie Structurale (IBS) – UMR5075 (CNRS/CEA/UGA), Grenoble (France) Bacterial cell division...



FELLOWSHIPS / FPI / PREDOC 07/12/2016

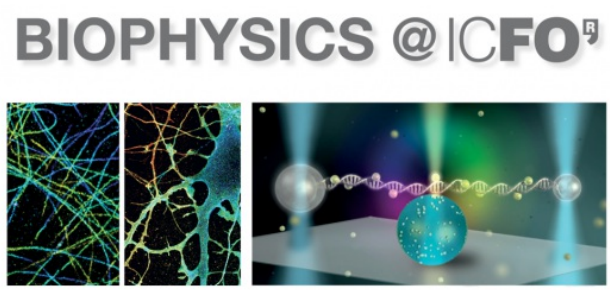
FPI-MINECO Fellowship at Structural Biology Unit – CIC bioGUNE

4 years Ph.D. position funded by FPI-MINECO from 2017 to 2020 The position is currently available at the Structural Glycobiology Group, Structural Biology Unit, CIC...

JOBS / POSTDOC 14/11/2016

Postdoctoral position in 3D nuclear organization

Applications are opened for a postdoctoral position at the Spatio-Temporal Organization of the Nucleus laboratory, at the FIRC Institute of Molecular Oncology – IFOM, Milan...



CALLS / JOBS / POSTDOC / PREDOC
26/10/2016

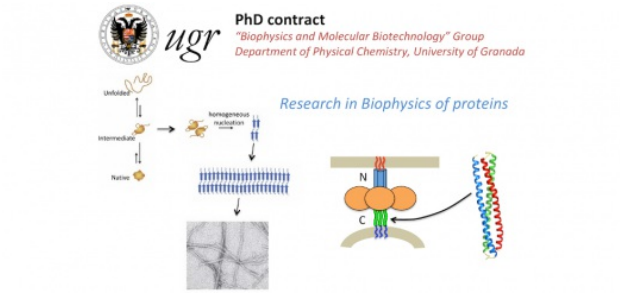
PhD and Postdoc Positions at the Institute of Photonic Sciences

Attractive opportunities to young scientists The Institute of Photonic Sciences – ICFO, a world-class multidisciplinary research centre located in Barcelona (Spain) is expanding its activities...

JOBS / POSTDOC 19/10/2016

Postdoc Contract / Laboratory of Neuroscience

El Laboratorio de Neurociencia, ubicado en el Centro de Investigaciones Biomédicas – CINBIO de la Universidad de Vigo busca un investigador joven y bien formado...



JOBS / PREDOC 04/10/2016

Predoctoral Position in Protein Biophysics

The group of Biophysics and Molecular Biotechnology of the University of Granada is offering a predoctoral position to a highly qualified and motivated graduate student...