Faculty of Natural & Mathematical Sciences
Department Physics

PhD Projects in the Dept. of Physics

Biological Physics & Soft Matter Group (BPSM)

Chaperone-mediated mechanical protein folding

Supervisor: Prof. Sergi Garcia-Manyes

The functional state of a protein is intrinsically linked to its structural conformation; typically a fully folded protein resides in an active state whereas a misfolded structure leads to a protein void of function with potentially disastrous repercussions in both cellular homeostasis and disease. The cell has an ingenious system of molecular chaperones that not only prevents protein misfolding, but also promotes the procurement of the native state. Despite the fundamental importance of this process, the precise mechanisms by which chaperones recognise misfolded proteins and eventually lead to efficient folding remains largely elusive. In order to gain insight into this molecular interplay we need tools capable of capturing the dynamic interaction of individual chaperones as the protein conformationally evolves into the native, folded state. In particular, we are interested in understanding the structural intricacies defining the dynamic molecular binding between the chaperone and its substrates in the last stages of folding. This PhD project aims at using a cohort of single molecule mechanics approaches (atomic force microscopy and magnetic tweezers) in order to understand the molecular mechanisms that govern chaperone mediated protein folding.

Ref: Perales-Calvo, J., Giganti, D., Stirnemann, G., Garcia-Manyes, S. «The force-dependent mechanisms of DnaK-mediated mechanical folding» Science Advances (2018) 4, 2.

Mechanobiology at the single cell level

Supervisor: Prof. Sergi Garcia-Manyes

Cells are subjected to different type of forces such as compression and tension, which are mainly induced by extracellular matrix, neighbouring cells and fluid flow. These mechanical stimuli are able to trigger activation of genes involved in differentiation, migration and proliferation. Recently the nucleus has been described as a possible mechanosensor, but the molecular mechanisms whereby mechanical signals result in gene expression are far to be completely understood. Using a combination of cutting edge techniques such as large-scanning AFM and magnetic tweezers, both coupled with a fluorescence microscopy, we aim at investigating the effect of compressing and stretching forces on the rate of nuclear shuttling of an array of mechanically activated transcription factors, including myocardin-related transcription factor (MRTF-A) or YAP. Overall this project would help us understand the contribution of tension and compression forces on activation of gene transcription.

Ref: Elosegui-Artola, A., Andreu, I., Beedle, A.E.M., Lezamiz, A., Uroz, M., Kosmalska, A., Oria, R., Kechagia, J., Rico-Lastres, P., Le Roux, A., Shanahan, C., Trepat, X., Navajas, D., Garcia-Manyes, S., Roca-Cusachs, P. «Force triggers YAP entry by mechanically regulating transport across nuclear pores» Cell (2017), 171, 1-14

Nanomechanics of Collagen

Supervisor: Dr Patrick Mesquida

Collagen is a structural protein that forms microscopically small fibrils in all vertebrates. These fibrils constitute the main component of many tissues, ranging from skin and bone to eyes. They are essential to maintain the mechanical strength and shape of these tissues. Because collagen fibrils are inherently biocompatible and can easily be processed, collagen fibril-based synthetic materials have been identified as potential scaffold materials in tissue-engineering. Such scaffolds are to be implanted in the living organism. They are necessary to grow new tissue and organs and are vital in the treatment of burn victims.

To function properly, it is important that the mechanical properties of scaffold materials are finely tuned and maintained to match those of natural tissues. This is normally performed by various techniques such as incubation with cross-linking agents, oxidisers, or controlled exposure to ultraviolet light. However, not enough is known about how these treatments influence the mechanical properties of collagen fibrils under various natural conditions.

In this project, we will use Atomic Force Microscopy to investigate the mechanical properties of collagen fibrils on the nanometer scale. We are looking for a highly motivated candidate with a first degree in Physics, Materials Sciences, Mechanical Engineering, or related fields.

You must have the willingness to work experimentally. Lab experience, for example gained in an experimental final-year project in your undergraduate degree is a great plus.

FRAP FLIM FAIM – an integrated multimodal fluorescence microscopy technique to study diffusion in cell membranes

Supervisor: Prof Klaus Suhling

Collagen is a structural protein that forms microscopically small fibrils in all vertebrates. These fibrils constitute the main component of many tissues, ranging from skin and bone to eyes. They are essential to maintain the mechanical strength and shape of these tissues. Because collagen fibrils are inherently biocompatible and can easily be processed, collagen fibril-based synthetic materials have been identified as potential scaffold materials in tissue-engineering. Such scaffolds are to be implanted in the living organism. They are necessary to grow new tissue and organs and are vital in the treatment of burn victims.

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Experimental Particle & Astroparticle Physics

Neutrino Oscillations at the T2K and Hyper-Kamiokande Experiments

Supervisor: Dr Jeanne Wilson

Measuring leptonic CP violation is a key ingredient to explain the current matter-antimatter asymmetry according to Sakharov's conditions, which could be achieved from the study of neutrino oscillations. Key experiments in the measurement of CP violation in neutrinos are T2K, currently taking data, and Hyper-Kamiokande, planned for the next decade. This PhD project will directly contribute to the challenging CP violation measurement at T2K, investigating methods to decrease the uncertainties related to the interactions of neutrinos with the detector. The analysis will focus on near (ND280) detector data analysis to develop new selections and improve the fits that allow us to extrapolate from near to far detector flux expectations. In addition, it will involve important contributions to R&D for the Hyper-Kamiokande experiment, in particular for the design and testing of the outer detector veto instrumentation. The successful PhD student will become a full member of the T2K and Hyper-Kamiokande international research collaborations, participating in detector operation service work and collaboration meetings. They will attend the University of London Particle Physics Postgraduate Lecture Course during their first year.

CP Violation at the T2K and Hyper-Kamiokande Experiments

Supervisor: Professor Francesca Di Lodovico

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New physics search from High Energy Astro-Neutrinos

Supervisor: Dr Teppei Katori

The IceCube Neutrino Observatory, at the South Pole, Antarctica, is designed to detect high-energy astrophysical neutrinos. These high-energy astronomical messengers provide information to probe the most violent astrophysical sources. An array of 8,160 digital optical modules (DOMs) are distributed in the antarctic ice to cover roughly 1 kilometre cubic volume, making IceCube the largest neutrino detector in the world. During this Phd, you will join the King's IceCube group, supervised directly by Dr Katori, working on the analysis of high-energy astrophysical neutrinos and looking for new physics from the astrophysical neutrino sample. The King's group is also actively working on phenomenology related to astrophysical neutrinos. The successful PhD student will attend the University of London Particle Physics Postgraduate Lecture Course during their first year and will also have the opportunity to work closely with the University of Wisconsin-Madison (UW-Madison) group.

Photonics & Nanotechnology

Simulation of electromigration using stochastic calculus

Supervisor: Samjid Mannan

This project aims to use a stochastic calculus based approach to solve the governing equations of electromigration. Finite element techniques are traditionally used to solve the equations that govern atomic movement in electromigration. However there are theoretical arguments that suggest that the stochastic calculus approach may be more powerful in this case, since electromigration causes the initially simple geometry to become ever more complex due to the voids formed by atomic transport in the presence of high electric current density and temperature gradients.

PhD in Novel Nanophotonic Phenomena

Supervisor: Dr Francisco Rodríguez Fortuño

The equations of electromagnetism, governing the behaviour of light and all other electromagnetic fields, exhibit truly intriguing properties when the size of material structures are comparable to or even smaller than the wavelength of light. These include novel effects and properties that are being uncovered only in very recent years, such as the spin-momentum locking of evanescent waves, the quantum spin Hall effect of light, and the complex underlying structure of the electric and magnetic fields at subwavelength scales enabling fascinating interference phenomena. On top of uncovering these novel properties, our group's philosophy is to find new applications based on them. In the past we have worked on advances in nanoscale light polarimeters, optical nanorouters, mechanisms for novel optical forces, nanoscale optical antennas with tuneable polarization, discovery of novel sources of light such as the Janus dipole, ultra-sensitive position sensors, and even proposing new exotic Casimir force effects.

Attosecond control of high harmonic generation process.

Supervisor: Amelle Zair

High harmonic generation (HHG) is the only non-linear process involved in light matter interaction that leads to the production of attosecond pulses. Controlling the electronic quantum paths in HHG is the only way to control the production and to enable a sustainable attosecond source for time resolved measurements of the fastest process in matter. In the project we will explore new approaches to control these quantum paths by employing combination of strong femtosecond laser field of multi-colour, multi polarisation and spatial shaped.

Filamentation sensing ultrafast dynamical process.

Supervisor: Amelle Zair

When an femtosecond laser field strongly interact with matter exceeding several critical power value for self-modulation, an equilibrium between non-linear effects can produce a plasma channel which unable laser pulses to propagate very long distances. This phenomena is called filamentation. In the filament produced femtosecond pulses experience Kerr effects and multiphoton ionization which change their properties. We used in particular filamentation to post-compress these femtosecond pulses to few cycle regime in a large range of wavelengths. In this project we will study a new route for filamentation while it is driven by complex laser field and in new materials such as liquid phase.

Theoretical Particle Physics & Cosmology

Non-Hermitian extension of the Standard Model for Particle Physics

Supervisor: Jean Alexandre

The consistency and phenomenological predictions of non-Hermitian extensions of the Standard Model for Particle Physics are studied analytically. Few recent articles published by the supervisor are:

J. Alexandre, J. Ellis, P. Millington and D. Seynaeve, ``Gauge invariance and the Englert-Brout-Higgs mechanism in non-Hermitian field theories''

Phys. Rev. D 99 (2019) no.7, 075024

J. Alexandre, J. Ellis, P. Millington and D. Seynaeve,

``Spontaneous symmetry breaking and the Goldstone theorem in non-Hermitian field theories''

Phys. Rev. D 98 (2018) 045001

J. Alexandre, P. Millington and D. Seynaeve,

``Symmetries and conservation laws in non-Hermitian field theories''

Phys. Rev. D 96 (2017) no.6, 065027

J. Alexandre, C. M. Bender and P. Millington,

``Non-Hermitian extension of gauge theories and implications for neutrino physics''

JHEP 1511 (2015) 111

Projects with Diego Blas

Supervisor: Diego Blas

Project 1) The aim of this project is to investigate two aspects of theories that violate Lorentz invariance. First, to clarify the gravitational collapse in these theories and other aspects of black holes. Do these theories solve some of the puzzles of General Relativity? Second, to investigate how one can recover Lorentz invariance at low energies in these theories.

Project 2) The aim of this project is to study how the recent developments in quantum technologies can help us to detect new phenomena beyond the standard model of particle physics.

Project with Malcolm Fairbairn

Supervisor: Malcolm Fairbairn

I am looking for a theory PhD student to work at the intersection of particle physics, astrophysics and cosmology. Typically I prefer a student to work on a variety of areas in order to gain the skills necessary to be a successful theorist in the modern environment. Subjects I am currently engaged in include probes of axion dark matter using strong lensing and dwarf galaxies, the use of dark matter detectors to constrain non standard dark matter particles, gravitational wave signals from phase transitions in the early Universe and the search for beyond the standard model physics in supernova explosions. I am also interested in students who are interested in generating their own projects and ideas, which I will support and help to develop. Successful applicants will be able to perform calculations with paper and pencil but also will be able to code. I aim to provide a supportive, positive environment for all students no matter what their sex, gender, sexuality or ethnicity.

New directions in the pursuit for dark matter

Supervisor: Chris McCabe

Chris McCabe's research lies in the area of astroparticle physics. This means that his research fuses ideas from particle physics, astrophysics and cosmology. Currently, Chris is engaged in projects to learn more about dark matter, which is prevalent throughout the universe. New theoretical and experimental ideas are needed to make progress. Chris is offering projects in the following areas:

1. to investigate new dark matter theories

2. to investigate new experimental signatures for dark matter in existing experiments

3. to investigate new dark matter experiments

Gravity and Cosmology in the era of Gravitational Waves

Supervisor: Mairi Sakellariadou

The advent of a new class of gravitational wave detectors, in USA and Europe, is changing gravitational physics in a dramatic way. The era of gravitational- wave astronomy began with Advanced LIGO's first detection of the collision of two black holes. Since then additional black hole collisions have been observed, and also the collision of two neutron starts was detected. The same way a microphone picks up the closest and loudest voices, detectors are most sensitive to loud collisions occurring in the relatively nearby Universe. Those (the majority) that are too faint or too distant to be observed individually, superpose to create what is called a stochastic gravitational wave background. And like a microphone is picking up the collective murmur of an audience, Advanced LIGO and Virgo may be able to detect the combined signal. Other, than collisions, gravitational events also contribute to the stochastic signal, and some were created during the earliest stages of the Universe (phase transitions, cosmic strings), hence much more before the beginning of stellar activity and the Cosmic Microwave Background.

In this project, we will study different sources that lead to a stochastic gravitational wave background, of either astrophysical or cosmological origin. In addition, we will explore the constantly increasing number of available data in order to constraint gravitational theories beyond Einstein's theory of General Relativity and particle physics models beyond the Standard Model. The student will be member of both the LIGO Scientific Collaboration and the LISA Consortium.

PT symmetric quantum field theory

Supervisor: Sarben Sarkar

At the boundary between Hermitian and non-Hermitian physics lies PT symmetric physics. A perfectly sensible unitary quantum physics can be generated through PT symmetric quantum mechanics. There is reason to believe that due to the effects of renormalization that many Hermitian quantum field theories are not consistent but show features consistent with PT symmetry. Some regard inconsistencies as a mathematical artifact which will disappear if a more complete physical theory is considered. In this project we ask whether PT field theory can be formulated self-consistently. This question is general and important and should be investigated properly; this project will do just that.

Theory & Simulation of Condensed Matter

Developing new computational approaches to tackle the quantum many-body problem in extended system

Supervisor: Dr George Booth

It is a curious fact that fully quantum mechanical predictions of the properties of isolated molecules can now be made with accuracy which rivals the most precise experimental spectroscopy techniques. However, when looking at extended systems, such as the interaction of a molecule with a solid surface, state-of-the-art computational approaches can often not even reach the accuracy required to deduce correct structures or interaction energies.

The aim of this ambitious research is to make progress in this area – to transfer the accuracy of quantum chemical approaches to the setting of extended systems, by development of new approximations and techniques which use the electronic wavefunction as the central quantity of the simulation. The wavefunction, despite being the first quantum variable which is introduced, is almost entirely neglected within computational simulations of extended systems. This is because of the exponentially large amount of information required to specify it, which has meant that alternatives such as the electron density has generally been used instead.

However, most of this complexity is artificial. For example, within insulating systems, the correlation length between electrons decays exponentially, and so approximations based on locality of electrons or embedding of correlation effects can be introduced, rendering it a tractable computational object. Additionally, parts of the wavefunction have a universal, analytic form (such as when two electrons occupy the same point), and so these parts of the wavefunction can be considered known, and removed from the required parameterization. Furthermore, clever optimization strategies can be developed, including Monte Carlo sampling of the wavefunction, and compact functional forms of the wavefunction, which can dramatically increase the potentiality of this approach.

These new ideas will be developed and then applied to real systems of significant technological interest, where current techniques are lacking, such as correlated transition metal oxide materials, and organic photoactive molecular crystals.

The project will have a large programming component, where these new methods will need to be coded and tested, before potential optimization for use on supercomputing resources. Furthermore, the successful candidate should have a strong background in modelling techniques and quantum many-body physics and/or chemistry.

For further information, please contact: Dr George Booth (george.booth@kcl.ac.uk)

Modelling binding and gating mechanisms in pentameric ligand-gated ion channels with enhanced sampling methods

Pentameric ligand-gated ion channels (pLGICs) are important neuroreceptors that mediate fast synaptic communication. They are involved in many neurological disorders, including Alzheimer's diseases, and are target sites for drugs and, in insects, for insecticides. However, due to their complexity and the limited structural information available, how they function at the molecular level is still far from being fully understood. The goal of this project is to study the activation mechanisms of prototypical pLGICs, focussing on the serotonin-gated 5-HT3 receptor whose structure has been recently resolved experimentally. This will be achieved by means of innovative computational methods that go beyond conventional molecular dynamics and ligand-protein docking, including the enhanced sampling metadynamics scheme to accelerate rare events and explore free energy landscapes. The specific questions that simulations will address are related to how ligands bind/unbind to and from the neuroreceptor, how the binding of ligands translates into the opening of the ion channel (eg through potential molecular switches), and the effects of mutations of key amino acids. The project will benefits from collaboration with experimentalists.

F. Comitani, C. Melis and C. Molteni, "Elucidating Ligand Binding and Channel Gating Mechanisms in Pentameric Ligand-Gated Ion Channels by atomistic simulations", Biochem. Soc. Trans. 43, 151-156 (2015). DOI: 10.1042/BST20140259 [mini-review]

'Nanofashion': designing metallic clusters at the nanoscale

Supervisor: Dr Francesca Baletto

In recent decades, metallic nanoparticles have contributed to developments in numerous scientific fields because of their unique physicochemical properties that make them extremely important for any technological application. Nonetheless, the strong relationship that intercourses between shape, size, and chemical composition –or simply geometrical features- and physicochemical properties is still not fully addressed, except for a few paradigmatic examples [1]. Measuring size and shape of nanometre clusters is a challenging task but numerical modelling are an important tools for driving experiments and to model/tailor/control nanoparticles from an atomistic point of view. Thus it appears clear that elucidating the relation between geometry and physicochemical properties with the aid of density functional and classical (empirical) numerical simulations is of primary importance for avoiding a "trail-and-error" approach in the design of metallic nanoparticles for catalytic, optical and magnetic applications. On this respect a huge contribution has been done recently by the introduction of the generalised coordination number for the mapping of active catalytic sites [2].

During this PhD, the candidate will gain expertise with both common ab-initio packages (e.g. Quantum Espresso, Onetep, and CP2K) and classical molecular dynamics –being actively involved in the development of the LOw-DImensional Systems molecular dynamics (LODIS) package that we are maintaining in the group, with features to calculate thermodynamics [2], growth [3] and structural transformations [4] in metallic and bimetallic nanoclusters. The final objective of the project is to find a route for the 'intelligent' design of metallic nanoparticles exploiting the dependencies of properties on geometrical features.

[1] P Strasser, Science, 349 (2015) 379

[1] F. Calle-Vallejo et al. Science, 350(2015) 185

[2] L. Pavan, F. Baletto and R. Novakovic, PCCP, 17 (2015) 28364

[3] I. Parsina and F. Baletto, JPCC, 114 (2010) 1504

[4] L. Pavan, K. Rossi and F. Baletto, JPC (2015), in press

The successful candidate should have a degree in physics or material science. For further details contact Dr Francesca Baletto (francesca.baletto@kcl.ac.uk).

Solving the problem of thermal energy waste by using quantum simulations

Supervisor: Dr Nicola Bonini

The project will focus on the design of new efficient materials for thermoelectric energy conversion, of crucial importance to harvest waste heat into electricity, or to provide an eco-friendly cooling technology.

The PhD student will use advanced electronic structure methods (density functional theory and its quantum many-body extension, DMFT and GW) to predict structural, electronic and thermal properties at equilibrium, as well as state-of-the-art methodologies to simulate transport phenomena at a quantum mechanical level.

These methodologies will be applied to novel sulphide compounds, a family of ecofriendly semiconductors that displays a rich structural variety and non-trivial promising electrical and thermal transport properties. No consistent theory for this class of materials is currently available. The goal will be to guide the synthesis of efficient materials and lead to the design of a thermoelectric device.

The project will be carried out as part of a collaboration with experimentalists at QMUL, who are experts in synthesis and characterisation of thermoelectric materials. The project will also benefit from the support of experts in the field of sustainable technologies, such as Kennametal, Johnson &

Matthey, European thermodynamics Ltd. The student will also benefit from interactions with the leading scientific software company Biovia. The successful candidate will be expected to liaise with the project partners.

The student should have a strong interest in some of the following topics: density functional theory, Green's function, quantum many-body effects, quantum chemistry, non-equilibrium physics, emergent behaviour.

Applicants must hold, or expect to receive, a first or upper second class honours degree (or equivalent) in Physics, Chemistry, Materials Sciences, or similar.

For further information, please contact: Dr Nicola Bonini (nicola.bonini@kcl.ac.uk)

Vortex Beams and Optical Metasurfaces

Supervisor: Carla Molteni

A PhD studentship is available to EU students starting from October 2019 or as soon as possible thereafter to work on complex vortex beams and optical metasurfaces within the framework of the ERC Advanced grant of Professor Anatoly Zayats. The project involves design, nanofabrication and optical studies of metasurfaces to control complex optical beams for a wide range of linear and nonlinear photonic applications. The project will be an experimental project involving fabrication and optical characterisation of metasurfaces, with applications in light polarisation control. We are looking for candidates with a strong background in optics and hands-on experience in optical laboratories. Knowledge of and experience in one or several of the following fields will be an advantage: optical vortex beams, ultrafast lasers, optical metasurfaces, optical forces, polarisation measurements, near-field optics, nanofabrication and numerical modelling

These PhD projects involve the application of atomistic computer simulations, including enhanced sampling methods, to study anti-oxidant effects in green tea catechins, mechanical properties of proteins, the interplay between amorphisation and crystallisation in pressure induced-structural transformations in nanomaterials and the mechanisms of crystal growth in ice and organic crystals. For information please contact Prof. Carla Molteni at carla.molteni@kcl.ac.uk.

P25: Out of Equilibrium Dynamics of Metallo-proteine at the single Bond Level

Primary Supervisor: Professor Carla Molteni

Secondary Supervisors: Dr Cedric Weber and Dr Sergi Garcia-Maynes

Metallo–proteins are ubiquitous in biology and important in many essential functions, from respiration to photosynthesis. One of the simplest example is haemoglobin, playing an essential role in mammal respiration. In vivo, many of these proteins are subjected to mechanical stress. However, the underlying mechanisms through which mechanical force affects the dynamics of metallo-organic bonds in the biological environment are still far from being understood. We plan to develop theoretical and computational tools to investigate the role of metal ions (namely Zn, Fe and Cu) in the non-equilibrium free energy landscape of the protein unfolding under applied force. Simulations will directly complement single molecule force spectroscopy experiments on paradigmatic examples to measure the bond breaking force. We will combined steered molecular dynamics and metadynamics with a quantum mechanical treatment of the active metal centres. The quantum approach will be based on dynamical mean field theory, a recently developed technique which allows to capture subtle many body quantum effects. The obtained time dependent electronic properties will elucidate the role of metal centres in the unfolding process, which require beyond state-of-the-art methodologies.

This interdisciplinary project will provide crucial data and insights into the time-dependent properties of molecules under strain, such as the single bond distortion and bond rapture in typical metallo-protein systems.