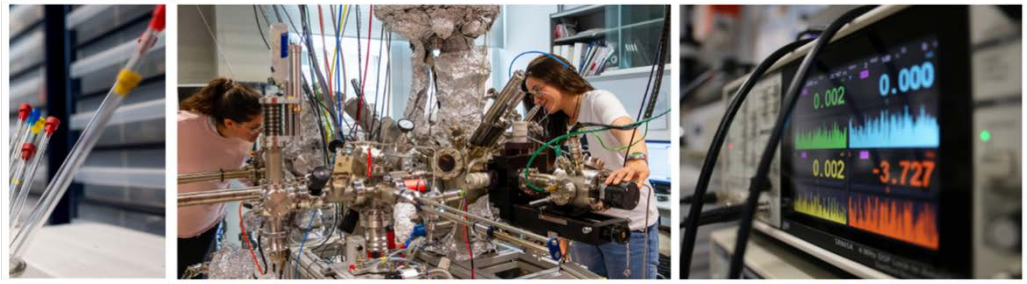

MASTER THESIS OFFER 2021/2022

1. **Fluorescent Single-Chain Nanoparticles for Sensing and Bioimaging Applications**
2. **New Photoactivated Synthesis Routes to Single-Chain Nanoparticles**
3. **High frequency phenomena in soft magnetic nanostructured materials**
4. **Cyclic polymers for biomedical application**
5. **Physics and Chemistry of Curved Crystal Surfaces: oxygen, carbon monoxide and carbon dioxide chemisorption and dissociation on stepped surfaces**
6. **Nanostructured materials for artificial photosynthesis**
7. **New Properties by Stacking Two-dimensional Graphene-like Material**
8. **Theory of optical nanocavity-molecule interaction**
9. **Anisotropic phonon polaritons in biaxial van der Waals materials**
10. **Anharmonic effects on the nuclei wave functions**
11. **Ultrafast adsorbate vibrational dynamics**
12. **Quantum transport and spin physics in graphene nanostructures**
13. **The Dzyaloshinskii-Moriya Interaction in ultrathin films**
14. **Enginneering of superconducting gap states**
15. **Nanowollastonite based Carbon-cured Concretes. A sustainable CO2 trappingsolution**
16. **Hybrid perovskites for photovoltaics – stability and degradation mechanisms**
17. **Electron simulator on the surface of Re(0001)**
18. **Angle Resolved Photoemission (ARPES) studies in magnetic Weyl semimetals and strongly correlated electron systems**
19. **Molecular dynamics study of Calmodulin**

1 Fluorescent Single-Chain Nanoparticles for Sensing and Bioimaging Applications

Single-chain nanoparticles (SCNPs) are the result of applying single-chain technology to individual polymer chains, giving rise to versatile folded/collapsed soft nano-objects of ultra-small size (2-20 nm). Significant effort has been spent in last years to endow SCNPs with useful and bioinspired applications for the fields of nanomedicine, bioimaging, biosensing, protein mimicry and catalysis, among others. This Master Thesis project is aimed to produce SCNPs with fluorescent properties of great interest for sensing and bioimaging applications.

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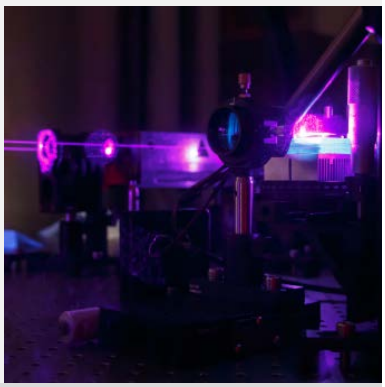
2 New Photoactivated Synthesis Routes to Single-Chain Nanoparticles



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3 High frequency phenomena in soft magnetic nanostructured materials

Phenomena like giant magnetoimpedance effect (GMI) and ferromagnetic resonance (FMR) in different families of soft magnetic amorphous, nanocrystalline and nanogranular metallic alloys have open new opportunities of research owing to the promising and, even, real technological applications. Such scientific research has dealt with several aspects concerning the intrinsic magnetotransport properties (i.e.: frequency range, intensity of the effect, magnetic field to observe possible maximum, noise…) as well as those related with microstructural (mainly amorphous or nanocrystalline) or geometrical character (wire, but these phenomena have been reported in glass-coated microwire, ribbon, multilayers, lantanide compounds and, therefore, high frequency magnetotransport phenomena are actually opening a new branch of research in soft magnetic materials. GMI and FMR combine the micromagnetics of soft magnets with the classical electrodynamics. Obviously, the different geometry and sample dimension together with the magnetic anisotropy lead to some differences in the GMI response like the range of frequency and the magnetic field dependence of the impedance curve with one or two peaks or even, it could be relevant the shape of the peak, etc.

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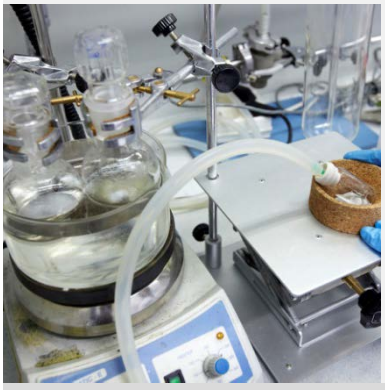
4 Cyclic polymers for biomedical applications

Cyclic polymers possess unique physico-chemical properties compared to their linear counterparts as a result of the absence of end-groups. In the past 60 years, examples of cyclic biomacromolecules have been found in nature, being circular DNA the first cyclic polymer to be studied in detail. The impact of these findings combined with the development of new synthetic tools has provided an increased motivation to further explore the synthesis, physical characterization and potential applications of cyclic polymers.

The aim of this Master Thesis is the synthesis of materials based on cyclic polyethers with potential biomedical applications, either in photodynamic therapy or drug release. The student will learn state-of-the art techniques for synthesizing and characterizing polymers with complex structures (MALDI-TOF MS, GPC with triple detection, NMR, FTIR, Raman spectroscopy, etc).



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5 Physics and Chemistry of Curved Crystal Surfaces: oxygen, carbon monoxide and carbon dioxide chemisorption and dissociation on stepped surfaces

Chemisorption and dissociation of gas-phase reactants are fundamental to understand heterogeneous catalysis. By exposing curved crystals of Pt, Pd, Cu, Ni, and Rh to O2, CO and NO we investigate the role of active step sites during gas-metal interactions for the most relevant catalytic processes, namely CO and NO oxidation. The work combines Valence Band and Core-level photoemission spectroscopy, and also implies the use of other Surface Science Techniques, namely LEED and STM and ARPES, all operating in Ultra-High Vacuum conditions.

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6 Nanostructured materials for artificial photosynthesis

The control over the materials structure down to nanoscale as well as their electronic structure are the most important requisites to develop artificial photosynthetic systems that through photocatalytic conversion can efficiently store light energy in chemical bonds. Especially important is the nanomaterials composition that defines light harvesting capacity and drive catalytic reactions via electron transfer. The aim of this project is the rational design and development of a hybrid nanoparticle-based photocatalyst using variety of sub-units such as molecules, supra-molecular complexes, plasmonic nanoparticles and quantum dots to be later assessed on a single particle level with sub-particle resolution. The project is multi-disciplinary and involves a variety of techniques, ranging from fabrication of nanostructures to their characterization using absorption, photoluminescence and Raman spectroscopy, fluorescence confocal lifetime microscopy imaging as well as fluorescence correlation spectroscopy. The material development and advanced characterization techniques will serve to study the fundamentals of photocatalytic processes related to photosynthesis with special focus on cofactor regeneration.

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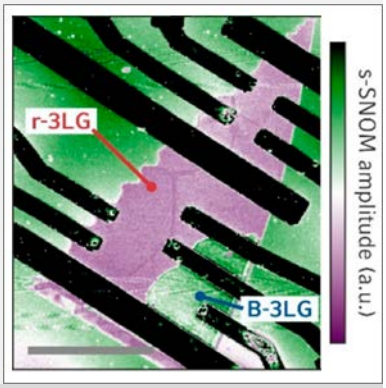
7 New Properties by Stacking Two-dimensional Graphene-like Material



New phenomena in condensed matter physics are based on two-dimensional materials. Although a single graphene looks promising for the future, research is today focusing on stacking several two-dimensional materials to form nanostructured materials made of carbon and other materials. The possibility to exfoliate materials and the existence of accurate experimental techniques to study single-layer materials supposed a big boost to study other layered materials. Currently much work is devoted to understand the recent finding of superconductivity in bilayer graphene. The aim of this project is to study the structural and electronic properties when having several layers of graphene either independently or sandwiched with other two-dimensional materials. During the master thesis project, the candidate will acquire knowledge in 2D materials, and gain expertise in using numerical tools, such as first-principles simulations calculations.

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8 Theory of optical nanocavity-molecule interaction

Plasmons in nanocavities and nanoparticles are collective excitations of conduction electrons at the surface of metals that give rise to resonant surface charge density oscillations at optical frequencies. These excitations induce extreme localization and enhancement of optical near fields, beating the diffraction limit and thus enabling the field of nanooptics. When a molecule is located in the proximity of a plasmonic nanoparticle, the electronic and vibrational excitations of the molecule can be dramatically enhanced and modified. The theoretical description of this effect requires the development of tools that involve methods from classical electrodynamics (to describe the optical response of a nanosystem), condensed matter physics (to describe the many-body properties of the plasmons), quantum chemistry (to describe the properties of molecules) and quantum nanooptics (to describe aspects of coherence of the plasmonic light). We plan to tackle some of these methodological aspects to improve our understanding of the nanocavity-molecule interaction.

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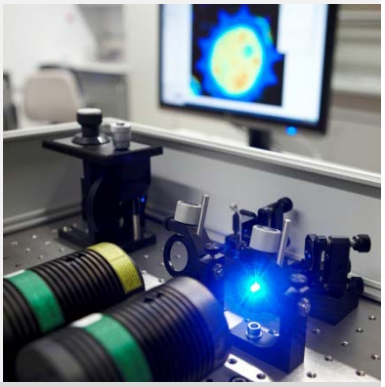
9 Anisotropic phonon polaritons in biaxial van der Waals materials



Low-dimensional van der Waals (vdW) materials have recently been attracting a substantial interest regarding photonics and optoelectronics applications since they support a variety of polaritons – oscillating dipolar excitations coupled to electromagnetic fields. Polaritons in vdW materials have different phase and group velocities in different directions, thus being strongly anisotropic. The project will study exciting exotic phenomena caused by the anisotropic polaritons, such as negative refraction, supefrocusing, slow light, etc.

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10 Anharmonic effects on the nuclei wave functions

In many cases, the inclusion of anharmonic effects in the nuclei dynamics is crucial to properly describe the physics of solids. This happens, for example, when light atoms are present, like in organic semiconductors and perovskites (of technological interest for photovoltaic and thermoelectric applications) and in hydrides (among which we have the highest critical temperature superconductors discovered so far). The stochastic self-consistent harmonic approximation (SSCHA) is an efficient method to include this effects in ab initio calculations. However, a full exploitment of this method to provide anaharmonic corrections to the nuclei wave functions is still missing. This could be very useful to correctly estimate quantities of physical interests, like the zero-point and the temperature-dependent electron energy bands (gap) renormalization, and the phonon-mediated optical transitions. The aim of the project is to develop the theoretical structure and the numerical implementation of the SSCHA method to obtain the anharmonic corrections to the nuclei wave functions. The first task will be the implementation of the method for simple 1D models with generic anharmonic potentials, with the aim of comparing the exact wave function (obtained by solving numerically the Schrodinger equation) with the SSCHA anharmonic wave function computed with higher and higher order corrections. By the end of the project, the candidate will acquire knowledge in numerical methods and in phonon anharmonicity (and in particular in the SSCHA method).

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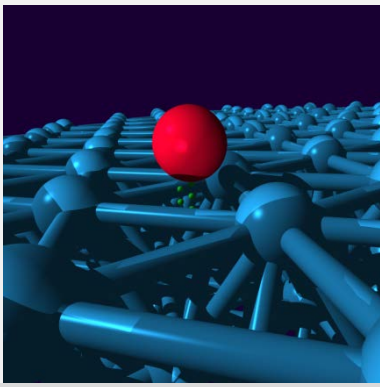
11 Ultrafast adsorbate vibrational dynamics



Ultrafast visible-infrared sum frequency generation (SFG) is a widespread technique that allows us to monitor the transient changes of adsorbates on surfaces. The recorded vibrational spectrum, characterized both by the frequency and the linewidth, brings information on the adsorption site, orientation of the adsorbed molecule, as well as on its interaction with the surrounding adsorbates and the surface. On metals, the lifetime of the vibrational excited adsorbates is strongly reduced due to the efficient excitation of electron-hole pairs. The aim of this master thesis project is to investigate from a theoretical point of view how this vibrational linewidth depends on various factors such as, the crystal face and surface coverage. The student will use two different approaches that are both based on density functional theory, namely, ab initio Langevin dynamics and density functional perturbation theory.

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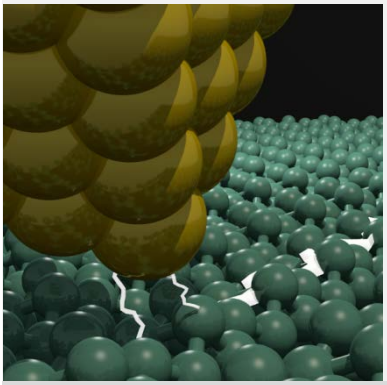
12 Quantum transport and spin physics in graphene nanostructures

Graphene nanostructures (GNS) show fascinating properties, including the possibility to develop intrinsic pi-paramagnetism from topological frustrations defined by their atomic structure. Nowadays synthetic chemistry and surface science techniques allow to produce and characterize such atomically precise GNS adsorbed on substrates. This situation makes GNS real and interesting candidates as elementary active components of a new generation of nanoscale quantum spintronic devices. In this theoretical project we will develop and apply computational approaches to predict properties of experimentally relevant compounds. A simple, yet highly successful, description of such systems is tight-binding and meanfield Hubbard models. We will compute topological properties and spin states of specific GNS and explore how they affect electron quantum transport through them, e.g., by injecting tunnelling currents from the tip of a scanning tunnelling microscope.



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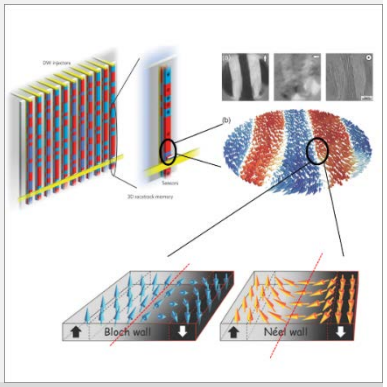
13 The Dzyaloshinskii-Moriya Interaction in ultrathin films

The spin-orbit interaction is at the origin of the antisymmetric exchange interaction between spins known as the Dzyaloshinskii-Moriya Interaction (DMI). Since it favours canted orientations of neighbouring spins, the DMI can result in exotic spin structures in the nanoscale that show chirality, i.e. handedness, such as spin spirals and skyrmions. This property of chirality is the foundation for many spin-based technologies.



Inversion symmetry breaking is a necessary condition for DMI. Therefore, we often find it localized at surfaces and interfaces. In the case of a layered heterostructure, if the layers are thick enough, the interfacial DMI contributions are essentially two-dimensional and independent of each other. This is not the case in the limit of ultrathin layers, where perpendicular chiral interactions are not quenched. As a consequence, screw-like rotating spirals and lateral displacement of skyrmions are predicted. During this Master Thesis project, we will study the DMI in this ultrathin limit by means of ab initio calculations. Our goal is to determine the DMI at the atomistic level, i.e. to have access to the tensorial exchange coupling constants themselves, and to understand the DMI dependence on the electronic structure.

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14 Enginneering of superconducting gap states

The subject of this master's work is the study of in-gap states in superconductors when mangetic impurities are present on its surfaces. This is part of the on-going experimental and theoretical effort of the group Quantum Phenomena on Surfaces at CFM-MPC. The aim of the study is to be able to generate electronic structure with increasing complexity as magnetic impurities are manipulated with a scanning tunneling microscope to create magnetic nanostructures. This strategy is what recently has benne term as reserach on "Designer Quantum States". The idea is to be able to create new states of matter that have special properties by marrying topology and quantum entanglement. This is particularly easy on superconductor susbtrates because their gound state is already a complex many-body entangled state. The object of the master is two-fold. First work with Bogolioubov-de Gennes equations to compute intricate in-gap electronic structure. Second porpose experiments that can be performed in an STM setup.

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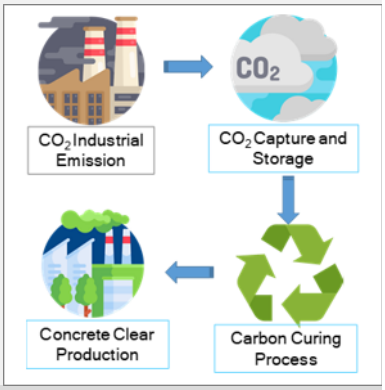
15 Nanowollastonite based Carbon-cured Concretes. A sustainable CO2 trapping solution



Cement industry is responsible for more than the 8% of total anthropogenic CO2 emissions to the atmosphere. It is not surprising that new cement formulations and production procedures are being sought after. In this context, a new family of cement-based materials have recently emerged: The Carbon-cured Concretes (CCC). Differently to normal cement based materials which need water for being cured and gaining strength, the Carbon-cured Concretes employ CO2 for triggering the carbonation of wollastonite (CaSiO3) minerals to form a solid cementitious matrix. Needless to say that the feasibility of CCC technology for trapping CO2 depends very much on the availability of wollastonite (CaSiO3). In this project, nano-wollastonite minerals will be produced by Supercritical Fluid (SCF) technology, following a recipe already proved as successful in a joint collaboration between the University of Bordeaux and the CFM.

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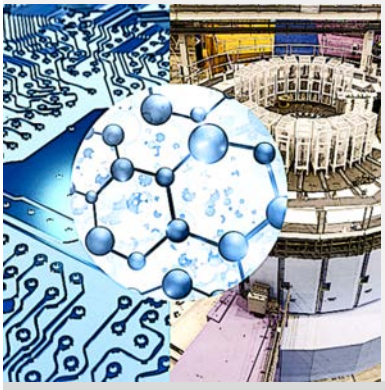
16 Hybrid perovskites for photovoltaics – stability and degradation mechanisms

Hybrid perovskites constitute a new class of energy materials whose photovoltaic response already exceeds 25%, *on par* with current (yet far more costly) silicon-based technologies. As such, these soft molecular solids offer the exciting prospect for the large-scale production of cheap, efficient, and flexible next-generation solar cells. Beyond their exceptional ability to harness the power of the Sun, they are also finding new applications in optoelectronics, quantum technologies, sensors, or memory devices. At present, the primary hurdle for their widespread use relates to their poor structural and chemical stability, also making the discovery of new candidates with improved performance a largely blind and labour-intensive endeavor. As part of wider research efforts using state-of-the-art experimental and computational techniques, the student will explore the physico-chemical mechanisms underpinning the stability and degradation of these materials under realistic conditions, with a view to attaining a detailed understanding of these processes at the atomic and molecular levels.



Contact: **Felix Fernandez-Alonso**
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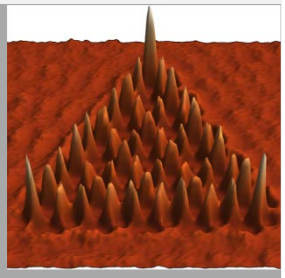
17 Electron simulator on the surface of Re(0001)



The electron quantum simulator is a particular type of analogue quantum simulator that can be used as a testbed for specific properties of quantum materials [1]. The electron quantum simulator has been studied by considering the surface states of Cu(111) and pattering a lattice by placing with the atomic precision various atoms or molecules [2,3]. In the past years, it has been employed for investigating, among the others, fractals, quasi-crystals and higher-order topological insulators [4-6].

In this project, we will study the realization of artificial lattices on the surface of Re(0001) [7]. The goal is to extend the concept of the electron quantum simulator to the realm of materials with spin-orbit interaction. The project will be developed by using the muffin-tin and the tight-binding methods. The work will be performed in collaboration with the experimental group of Ingmar Swart at the University of Utrecht].

References:

[1] R. P. Feynman, Int. J. Theor. Phys. 21, 467 (1982).
[2] H. C. Manoharan, C. P. Lutz, & D. M. Eigler, Nature 403, 512 (2000).
[3] K. K. Gomes et al., Nature 483, 306 (2012).
[4] S. N. Kempkes et al., Nat. Phys. 15, 127 (2018).
[5] L. C. Collins et al., Nat. Commun. 8, 15961 (2017).
[6] S. N. Kempkes et al., Nat. Mater. 18, 1292 (2019).
[7] L. Schneider et al., Nat. Commun. 11, 4707 (2020)

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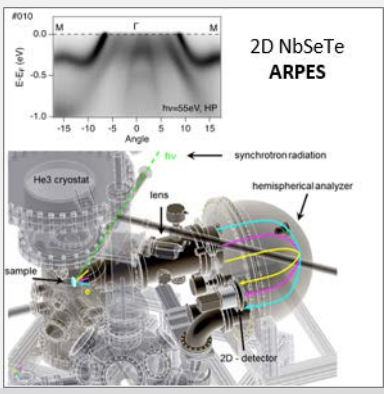
18 Angle Resolved Photoemission (ARPES) studies in magnetic Weyl semimetals and strongly correlated electron systems



The rapid progress in material synthesis and ab initio calculations has allowed the discovery of new materials that host novel physical phenomena and topological properties. Among those, Dirac and Weyl fermions are of current interest due to its possible applications in electronics and computing due to the high mobility of charged Weyl fermions. In particular, the Weyl fermions at zero energy correspond to points of bulk band degeneracy, the Weyl nodes (or Fermi points), that are separated in momentum space, and present distinct chiralities, either left-handed or right-handed. When the Weyl nodes happen at the Fermi surface, the Weyl points may get nested and a gap opens, breaking the bulk band degeneracy. The term Weyl driven charge density wave has been coined to name those materials where a Weyl driven gap opens at the Fermi surface.

The present project addresses the experimental realization of Weyl driven charge density wave materials by studying the electronic and phononic band structures by means of angle resolved photoemission (ARPES) and Inelastic X-ray scattering (IXS). He/she will study the band topology of magnetic Weyl semimetals and CDW systems by means of synchrotron ARPES with especial emphasis in $(TaSe_4)_2I$, $NbTe_4$, $MnGeO_3$ and 122 Co, Ni and Ru pnictides. The candidate will acquire skills in synchrotron radiation in several facilities around the world: Barcelona, Paris, Berlin, New York, Chicago, San Francisco, Osaka, etc and will get introduced to the ARPES and IXS techniques. He/she will have the opportunity to lead the experiments, analyze the data and interact directly with theoreticians.

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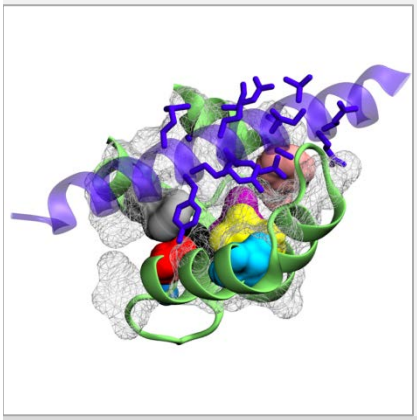
19 Molecular dynamics study of Calmodulin

The complete resolution of the sequence of the human genome in 2016 has been a huge milestone that continuously reveals causal relations among pathologies and gene signaling. Moreover, the latest advances of experimental techniques, such as nuclear magnetic resonance, provide a direct access to 3D maps with atomic resolution of the proteins that form cell membranes. This new accessible structural information has become a revolution in biological sciences for the design of new drugs that improve the well-being of humans. Remarkably, 60% of the commercial drugs act precisely on the proteins located at the cell membranes. With this scenario in mind, physical models that mimic atomic interactions within the proteins and their posterior time evolution through molecular dynamics provide a very powerful tool for the prediction and comprehension of membrane phenomena. Theoretical simulations of proteins serve as a guidance for the design of new drugs and help understanding the enormous amount of experimental information available. In this Master Thesis we shall consider the Kv7.2 channel of neuron membranes — a potassium voltage-gated channel located in human neurons —whose functioning relies in a potential difference induced by calmodulin (CaM). By means of All-atom simulations, molecular dynamics and coarse grain models, we would like to validate two claims regarding the behavior of the secondary structure of the IQ motiv of the channel: 1) Both wild type and mutant can form stable helices without the ribosome; 2) Wild type can form an alpha helix at the ribosome whereas the mutant cannot.



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