**Strongly Correlated Electrons in Quantum Materials and in Far from Equilibrium Nanostructures**

Funding Agency: Spanish Ministry of Science and Innovation.
Principal Investigator: Jaime Merino.

Description:

The main goal of this project is to study the novel phases of matter that can appear in materials in which strong electron-electron interactions play an important role in determining their electronic properties. We concentrate on several important aspects which occur in such strongly correlated systems: possible novel states of matter close to quantum phase transitions, geometrical frustration effects in Mott insulators and far from equilibrium phenomena in nanostructures. Our proposal is relevant to the understanding of electronic properties of organic materials, heavy fermions, transition metal oxides and nanostructures with potential technological impact in the future. It also includes the development of theoretical approaches that can describe correlated insulators under external fields.

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**Quantum and Nonlinear Phenomena in Plasmonics**

Funding agency: Spanish Ministry of Science and Innovation
Duration: January 2012-December 2014
Principal Investigator: Francisco J. Garcia-Vidal

Description:

We study from a theoretical perspective several electromagnetic phenomena that appear in structured metals.
More precisely, we address the following topics:

Study of extraordinary optical transmission through apertures in the presence of resonant molecular systems: strong coupling between molecules and plasmons, and analysis of the yet unexplained the transmission resonance induced by the molecular absorption band.

Metallic metamaterials: exploration of the geometrical impedance concept in the optical regime, and study of whether added non-linear materials can reduce absorption losses.

Optimization of SP based optical devices, as hole arrays for use in IR absorption spectroscopy, and apertures flanked by surface corrugations for miniaturized detectors.

Exploration of the transferability of plasmonic phenomena to sound waves.

Graphene plasmonics: study of the optical properties of graphene, especially those related to the bound electromagnetic modes that this material supports.

Non-linear phenomena and lasing: study of the optical effect associated to the intrinsic non-linear response of metals, and development of theoretical framework to treat simultaneously the dynamic of optical-gain materials and the electromagnetic field in plasmonic structures, for its application to pumped systems, solitons in waveguides and lasing in metallo-dielectric systems showing strong field enhancement.

Transformation optics for plasmonics and its application to the study of non-local effects.

Quantum plasmonics: tailoring effective interactions between quantum emitters via surface plasmons, study of the quantum noise of surface plasmons under excitation with non-classical fields and ways to generate single plasmons and entangled pairs.

NANOQUO - Nanostructures for Quantum Optics
Funding Agency: Spanish Ministry of Science and Innovation.
Principal Investigator: Carlos Tejedor

Description:

This project is devoted to the experimental and theoretical study of condensed matter nanostructures as components for quantum optical information processing. Quantum information processing is based on a direct consequence of the quantum superposition principle: a system composed by subsystems has states that can not be factorized in products of states of its components. This nonseparability, labelled as entanglement, is at the heart of quantum cryptography, quantum teleportation or other quantum operations. Pairs of photons are the usual candidates for supporting and transmitting quantum information encoded in photonic entangled states. The production “on demand” of such pairs is a very active field of research and is the first task of this project.

Apart from manipulating photons, we investigate other bosonic quasi-particles as candidates for performing quantum states engineering for transmission and support of information. In particular, exciton-polaritons in semiconductor nanostructures and plasmon-polaritons in metallic nanostructures.

Our second task is the study of exciton-polaritons. In this case, our interest is not only to look for entangled states but also to engineer novel quantum states macroscopically coherent. Under suitable pumping conditions, exciton-polaritons might undergo a transition to a novel collective state: a superfluid behaviour in out-of-equilibrium conditions.

In our third task of this project we investigate plasmon-polaritons in hybrid metal-semiconductor nanostructures as the basic ingredient of a very promising but not yet developed field: quantum plasmonics. On top of the fundamental interest of this new field, our motivation comes from the fact that plasmon-polaritons fulfil two essential requirements for quantum information processing as tunable qubit-boson coupling and controllable dissipation.
Correlated Electrons in Hybrid Nanostructures: From Transport Properties to Quantum Information Processing

Funding Agency: Spanish Ministry of Science and Innovation (FIS2011-26516).
Duration: January 2012 – December 2015.
Principal Investigator: Alfredo Levy Yeyati.

Description:

This project aims to study theoretically different phenomena associated with electronic transport in hybrid nanostructures. The project includes the following research lines:
- Correlation effects in molecular junctions.
- Andreev bound states in superconducting junctions.
- Splitting of Cooper pairs in double quantum dot devices.
- Electron transport in topological insulators.

Theoretical Description of Wave Propagation in Magneto-Plasmonic Nanostructures
The main objective of this project is to investigate theoretically the optical properties of metallic nanostructures with both plasmonic and magneto-optical (MO) activity. The major technical goal is the generalization of the scattering matrix approach to describe the magneto-optical effects in nanostructured magneto-plasmonic systems. This method will then be applied to address three basic challenges in the field of magneto-optics:

The interplay between the extraordinary optical transmission and the MO effects in metallic films with MO activity and perforated with periodical arrays of sub-wavelength holes.

The design and optimization of novel surface plasmon resonance biosensors based on the transverse magneto-optical Kerr effect in magnet-plasmonic nanostructures.

Analysis of the magneto-optical properties of hybrid systems formed by two-dimensional photonic crystals fabricated by means of self-assembly of colloidal particles which are deposited on multilayer metallic structures with MO activity.

Self-Assembling Materials: Theory and Simulation

The research project is in the field of soft materials. It further sub-divides in two parts, both dealing with self-assembling systems.

The density functional theory and numerical simulation of the phase behaviour and properties of suspensions of colloidal non-spherical particles. Focus is currently on two types of concave model colloidal particles: (a) hard lens- and bowl-like particles that show an intriguing phase behaviour featuring an entropy-driven competition between phase separation and clustering, in analogy with what happens in molecular systems forming micelles; (b) hard helical particles as a basic model for a range of natural and synthetic soft matter systems: from natural poly-nucleotides and peptides, to synthetic helical polymers, from bacterial flagella to colloidal helices.

Recent work proves the existence of a new chiral nematic phase in such systems, termed screw-like, along with new smectic phases that combine screw-like ordering with layering. Of major concern is the understanding of the subtle relationships between particle chirality and the chirality of the phases formed.

The design of improved semiconductive columnar liquid-crystalline materials for application in electronic devices, by the synergy of high level quantum calculations of intermolecular interactions, classical atomistic molecular dynamics simulations of the phase behaviour and kinetic Monte Carlo simulations of charge transport to predict structural properties, including structural fluctuations and defects, of these self-assembling materials and how these properties influence the one-dimensional charge transport characteristics.
The development of instruments and methodologies to explore the nanoscale is critical to expand our knowledge at the molecular level. That knowledge will eventually lead to technologies that have the ability to image, modify, characterize, interface and process nanoscale systems with a broad range of applications from nanoelectronics to clinical research and diagnosis. Force-for-future contains an integrated approach to develop a new paradigm in Force Microscopy (AFM) that will improve the spatial resolution and material properties sensitivity of the instrument at the molecular level in air, vacuum or liquid of a wide variety of materials from cells, proteins and semiconductors. Furthermore, the project will develop multiscale computational codes to convert experimental data at the nanoscale into relevant information about mechanical and electronic properties. At the same time, the project explores applications in two fields with promising technological or health implications: nanomechanics and biomedicine. In particular, the project will anticipate future applications of nano-microscopies in clinical diagnosis. The ability of the AFM for high resolution imaging of soft materials in physiological conditions makes this instrument as a potential candidate for clinical diagnosis.

Our SPMTH research group at UAM is going to develop protocols based on steered molecular-dynamics (MD) simulations with well-established classical potentials (AMBER), with the aim of understanding: (i) protein adsorption on surfaces; (ii) the connection between the local effective elastic properties measured with AFM and the real atomistic deformation mechanisms used by large proteins (like human antibodies) to release the stress created by the tip; and (iii) the role of water in the conformation of biological material and its atomic scale characterization with AFM.
Structure and Dynamics of Complex Fluids and their Interfaces

Funding Agency: Spanish Ministry of Science and Innovation.
Duration: January 2011 – December 2014
Principal Investigator: Enrique Velasco

Description:

The project focuses on a variety of fundamental problems in the structure and dynamics of complex fluids and their interfaces, problems that are central to the field of Soft Matter. We use theoretical tools based on statistical mechanics, together with numerical simulations. It is a coordinated project that includes various research groups that share common interests. One of the main objectives of the project is the formulation of connections between mesoscopic physics (hydrodynamics, effective models, etc) and the underlying (molecular) microscopic physics in a soft-matter context. The aims are within the boundaries of statistical physics and some of its interdisciplinary applications:

- Biophysically inspired problems, such as formation of protein filaments or description and dynamics of membranes and vesicles.
- Molecular scale dynamics of capillary waves in complex fluid surfaces and their hydrodynamics at the mesoscopic scale.
- The connection between molecular hydrodynamics and dynamic density functionals.
- Formulation of consistent coarse-graining theories for complex fluids.
- The structure and dynamics of polymers and colloids in a solvent and at interfaces.
- The formulation of models that bridge the gap between the microscopic and the mesoscopic description of liquid crystals containing topological defects.