

INP

INSTITUTE OF PHYSICS RESEARCH NETWORKS (GDR) IN 2022



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(GDR) is a native CNRS entity that brings current, fundamental scientific or European or international level. societal issues.

CNRS institutes concerned.

GDRs are established for a period of five teams comprising staff scientists, faculty, PhD students, post-doctoral fellows and - and private companies.

The main missions of a GDR are: to

The « Groupement de Recherche » organize a scientific community, often multidisciplinary, around a specific together and federates a scientific theme, while encouraging new partners community around an emerging, to join; to develop exchanges between original research topic. The CNRS' scientists within the network of Institute of Physics regularly initiates laboratories involved; and finally to set new GDRs on subjects related to up collaborative projects on a national,

In this regard, it is entirely possible While at the heart of the Institute of to intensify the collaboration of the Physics' science, these topics may scientific communities of the GDRs also interface with other scientific with industry, via the constitution of a fields. Such transdisciplinary GDRs are «partners' club» which, within a GDR, supported in association with the other allows for better mutual knowledge and the identification of common research topics.

years, renewable once, and are led by a The work of the GDRs in 2021 has director. They bring together research been affected once again this year by the health crisis, making face-to-face meetings more difficult: I would like engineers from CNRS research units as to sincerely thank the GDR leaders for well as institutional partners - such as their continuous efforts to maintain the universities, CEA, Inserm, Inra or Ifremer animation of the scientific communities in this context, and also thank those who are joining the GDR adventure.

This booklet presents, in the form of

summary sheets, the objectives and prospects of each of the research groups supported by the Institute of physics in 2022. In addition to presenting the research performed on diverse emerging topics, I hope that this booklet will entice new partners from other fields to bring their complementary scientific expertise to these GDRs for the benefit of all parties.

GDR ADN&G* ARCHITECTURE AND DYNAMICS OF THE NUCLEUS AND GENOMES

The mission of the **Architecture and dynamics of the nucleus and genomes (ADN&G)** research network is to bring together the French community involved in the study of nuclear organisation and interested in physical modelling. At the interface of physics and biology, the GDR ADN&G aims to understand the functional role of the organisation in physiological processes and associated pathologies by encouraging the emergence of of an integrated approach of the architecture of chromosomes and their dynamics on different size and time scales.

* Architecture et dynamique nucléaires et génomes







Experimental techniques of molecular and cellular biology Super-resolution microscopy Biotechnologies High-speed approaches Bioinformatics Statistical physics Numerical simulation 3D visualisation and animation techniques Physical modelling 2000 researchers involved within 50 laboratories

9 research topics

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PROSPECTS

The Architecture and dynamics of the nucleus and genomes research group (CNRS GDR «ADN&G») aims to work in a cooperative and united way, and to strengthen the links between teams working on the 3D organisation of genomes. It has the dual characteristic of being interested in the entire living world - eukaryotes, but also bacteria and archaea - and of focusing on physical and numerical modeling. This choice of approach opens up the unique possibility of considering nuclear organisation in the light of cellular differentiation and development, pathologies (cancers, infectious, chronic and neurodegenerative diseases) and the evolution of species. How are the universal functions fulfilled by the chromosomes of the entire living world implemented by the different types of nuclear organisation? According to which physical principles? How are certain mechanisms dysregulated and how do they lead to pathologies ? Which mechanisms have started to be set up but have remained at the beginning in some species (so-called «inchoate» processes) while they have ended up in others?

In addition to the immense scientific challenge of understanding the physiological nuclear organization and its pathologies, there is another challenge - that of supporting the teams concerned in the face of international competition. A collaboration dedicated to the same theme, financially supported by the National Institutes of Health (NIH), began in the United States in 2015 with the launch of the «4D Nucleome» program. Exclusively dedicated to the study of the architecture and dynamics of human cell nuclei, this multi-year program, with an annual budget of \$30 million, aims to take the lead in this highly competitive field. In order to have an international impact, we believe it is crucial that a similar initiative be set up in Europe. To this end, we would like to join our forces with other french research groups with related themes (CNRS GDRs Imabio and AQV) as well as other players in the various European countries. This initiative would be an excellent opportunity to develop the synergy that we have initiated and to highlight the strengths of our approaches. It would also be an excellent opportunity for the CNRS to influence the orientations of future European programs.

GDR BIOCOMP* HARDWARE IMPLEMENTATION OF NATURAL COMPUTATION

The mission of the **Hardware implementations of natural calculation (BioComp)** research network is to bring together and structure the French community working on the realisation of bio-inspired hardware systems. BioComp aims both to understand the mechanisms at work in biological systems in order to create new types of chips based on natural computation, and to build hybrid hardware architectures in order to better understand biology.

* Implémentations matérielles du calcul naturel







6 research topics

Neuromorphic systems

Artificial Intelligence

Bio-inspired computation, cognitive neurosciences and cognitive psychology

Biologically inspired information processing

Materials, physics and electronics for bio and neuroinspired computation

Neuro-inspired robotics



160 researchers involved within **60** laboratories

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PROSPECTS

There are many challenges in electronic systems inspired by the brain:

ENVIRONMENTAL

The IT industry already consumes more electricity than India because of the massive use of data centres, especially for running artificial intelligence (AI) algorithms. Neuromorphic systems can drastically reduce this electricity consumption, towards green AI.

ECONOMICAL

The applications of bio-inspired computing systems can be divided into two classes. The first is to accelerate and miniaturise AI for autonomous vehicles, robotics, prostheses, connected networks, etc. The second is to provide supercomputers to enable neuroscientists to run models of the brain.

SOCIETAL

The future development of AI requires changing the hardware on which these algorithms are supported. France is at the forefront of fundamental research in this field.

ETHICS

The development of this new electronics will change the way we interact with machines and raise many ethical questions. From the uses of these technologies, data protection, societal changes to the legal place of these artificial systems, many questions need to be addressed upstream.

SCIENTIFIC

Moving towards the realisation of bio-inspired hardware computing systems will enable scientific advances in all the fields concerned - neurosciences, mathematics, computer science and information processing systems architecture, microelectronics, nanotechnologies and physics.

To meet these goals, many challenges must be met:

INTERDISCIPLINARITY

This is a nascent research field, which to succeed must bring together researchers from physics to neurosciences via microelectronics and computer science.

HARDWARE IMPLEMENTATIONS

Nanoneurons and nanosynapses with low energy consumption, in tens of millions (10¹¹ neurons in the brain) must be produced, modelled, densely connected (10⁴ synapses per biological neuron), and adapted algorithms developed (challenge: unsupervised learning).

MODELS

Embedded AI systems require new models, less demanding in resources, capable of learning with very little data, tolerant to component imperfections, robust to catastrophic interference, and capable of performing multiple cognitive functions beyond pattern recognition (multisensory fusion, attentional or predictive circuits).

GDR CHALCO* CHALCOGENIDE MATERIALS: RESEARCH, DEVELOPMENT AND INNOVATION

The mission of the **Chalcogenide materials: research, development and innovation (CHALCO)** research network is to bring together the french community working at the forefront of science/technology around chalcogenide materials in a large variety of multidisciplinary fields. The CHALCO research group aims at structuring this community, on the french national level, to empower the different players to collaborate and interact beyond their own native field. This will be made possible by a vertical netting from fundamental research to industrial applications, and a transverse netting in the 4 identified fields: memories/neuromorphic, optical/photonic, thermal/energetic and spin-orbitronics. Linking all the knowledge/research operators from the fundamental research up to the industrial production will enable the emergence of new synergies in all the deep tech fields where chalcogenide materials are involved.

* Matériaux chalcogénures : Recherche, Développement et Innovation







7 research topics

Memories and neuromorphic applications

Optical and photonic applications

Thermal and energy applications

Spin-orbitronic applications

Theory, design and modeling

Production of materials

Advanced characterisations



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PROSPECTS

MEMORIES/NEUROMORPHIC APPLICATIONS:

The strategy on the european level is to develop a technological industrial sector able to manufacture embedded phase change memory (PCM) devices. These devices require improved storage capacities compared to current $Ge_2Sb_2Te_5$ PCM devices as they have to work in a more aggressive environment. All the aimed properties are rooted in the morphological and/or physicochemical properties of the thermally activated thin chalcogenide nanometer scale layer. We aim for the design, characterization and validation of new materials which can be effectively used in industrial processes. Furthermore, PCM memories are currently one of the best candidates for neuromorphic new computing schemes which may revolutionize the way computers work.

OPTICAL/PHOTONIC APPLICATIONS:

This field covers the development of new optical components with enhanced capabilities in the mid IR, non-linear and adaptative optics and computing domains. The main challenges are:

- Designing new bulk/nanometric materials with enhanced properties;
- Developing new synthesis, growth and shaping pathways;
- Implementing machine learning approaches to model the multiphysical properties of materials;
- Improving numerical tools based on harmonic approaches for the linear regime, and temporal approaches to study the nonlinear regime.

THERMAL/ENERGY APPLICATIONS:

This field is mainly divided in the following 3 sub-fields:

- Thermoelectricity: new materials with reduced thermal conductivity via doping/phase/nanostructuration. The band degeneracy, anisotropy, high anharmonicity-induced processes should result in an increased power factor. Design in new flexible devices using doped/low dimensional material/nanostructured;
- Photovoltaic applications: new solar cell materials with improved ecological properties compared to the current CdTe or the technology using rare element (CIGS);
- Batteries: all-solid-state batteries based on glass or glass-ceramics chalcogenides with increased ionic conductivity (à 10⁻⁴ to 10⁻³ S.cm⁻¹ diameter at ambiant temperature). Improving the solid/solid interface between the electrolyte and the active materials which also ensure a chemical and electrochemical stability of the electrodes.

SPIN-ORBITRONIC APPLICATIONS:

The spin orbit coupling allows the charge current to be converted in spin current and vice versa. They are 2 main type effects: the spin Hall effect (a volume effect) and the Rashba-Edelstein effect (in 2D or interfacial materials). The main challenges are:

- Measuring the interconversion charge/spin current in order to select the best chalcogenide materials ,taking into account industrial constraints;
- Integrate the selected materials in devices for spin-orbit reading and/or spin-transfer torque.

GDR COHEREX* SCIENCE WITH COHERENT X-RAYS AT 3RD AND 4TH GENERATION SYNCHROTRON SOURCES

The assignment of the **Science with coherent X-rays at 3rd and 4th generation synchrotron sources (CohereX)** research network is to gather the French community using coherent X-ray techniques for their research that spans from biological systems over cultural heritage materials and functional materials to the electronic and magnetic structure and dynamics of matter. CohereX aims to share the know-how and to foster the development of novel innovative studies and data analysis approaches, in particular, with respect to the unique opportunities offered at upgraded extremely brilliant synchrotron sources.

*La science avec les rayons X cohérents dans les sources synchrotron de 3^{ème} et 4^{ème} génération







Functional materials (ferroelectrics, magnetic materials, batteries...) Cultural heritage materials Biological systems Biominerals and biomimetic materials Dynamical fluctuations in complex materials High-energy coherent X-rays Big data and data management Machine learning for data treatment

8 research topics



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PROSPECTS

The continuous improvement of brilliance and coherent flux in modern synchrotron sources has led to the emerging of new techniques to probe physical and chemical properties of matter. Existing synchrotron facilities are presently undergoing major upgrades to extremely brilliant sources, increasing the available coherent flux by 1 to 2 orders of magnitude. This increased coherent flux significantly improves the sensitivity and helps to achieve very high spatial resolutions, potentially down to the atomic level. Also, the higher photon flux of coherent high-energy X-rays, that have a higher penetration power into matter, will facilitate the study of larger samples or within actual working environments. It will further increase the temporal resolution, eventually allowing physical processes to be measured at shorter timescales.

In a very competitive international environment, the French communities using coherent X-rays are well recognized. Fostering the discussion between members experts of different coherent X-ray techniques will lead to a most effective way of usage of the new opportunities at extremely brilliant sources. It will pave the way to innovative studies of the structure and defects of functional materials like ferroelectrics and magnetic materials and allow developing novel in situ and operando approaches, e.g. for catalysis or electrochemistry for battery applications with nanoscale resolution. It will further help investigating various physical phenomena such as damage in aluminium alloys (for aeronautics applications) at the submicron level and provide 3D multiscale characterization of new additive manufacturing processes with operando devices to mimic the process. In addition, biological imaging will be beneficial to eventually provide quasi-histological information on post-mortem tissues giving important insight about the 3D structure of intact organs or pathological tissues of any type. Moreover, innovative investigations of the multiscale thermo-hygro-mechanical behavior of natural cellulose fiber materials, the fluid/structure interaction during the processing of composite materials, and the monitoring of the behavior of high frequency systems will become possible as well as the dynamical fluctuations in complex materials with unprecedented temporal resolution.

A challenge for the coming years is the management and treatment of the big amount of data recorded during coherent X-ray experiments. It is thus essential that members of the community meet and discuss about artificial intelligence and machine learning in order to develop novel convolutional network-based algorithms for data analysis.

Nowadays, coherent X-ray techniques are niche methods. The grouping of the community will significantly increase the visibility. The GDR is further open to non-specialists to promote the interaction with other communities and the development of novel experiments and data analysis approaches and to bring coherent X-rays out of their niches and eventually make them a standard tool for imaging and studying matter. This GDR is also of importance regarding an eventual upgrade of the French synchrotron source SOLEIL and of the French CRG beamlines at the European Synchrotron ESRF.

GDR COMPLEXE* CONTROL OF WAVES IN COMPLEX MEDIA

The mission of the research network **Control of waves in complex media (COMPLEXE)** is to gather the French community involved in both fundamental and applied research in the field of the physics of waves in complex media. COMPLEXE aims to foster exchanges between opticians, acousticians, cold-atom physicists and seismologists, and focuses on fundamental aspects of the propagation of waves as well as on the development of novel methods for control and imaging of waves within complex media.

*Contrôle des ondes en milieu complexe





4 research topics

Methods of control, imaging and characterization of waves in complex media

Fundamental research on the mesoscopic aspects and the localization of waves in disordered media

Wave transport in correlated or nonlinear media

Waves as simulators of quantum or topological systems





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PROSPECTS

The GDR COMPLEXE gathers researchers coming from diverse fields but motivated by a common question; decipher and use the propagation of waves in "complex" media. In our daily environment, complex media are often more the rule than the exception: they are for instance materials that deviate from perfect crystals due to defects, heterogeneous biological tissues, emulsions or dense gases of particles. In these systems, the propagation of waves does not follow a straight line but is erratic. This process is a problem as well as a resource, because it makes imaging difficult but, on the other hand, it gives rise to original physical phenomena. The study of waves in complex media raises both fundamental and applied challenges, which lie at the heart of the interdisciplinarity of the GDR COMPLEXE.

CONTROL AND IMAGING

In a complex medium, controlling the propagation of waves or using them for imaging has long been considered hopeless. Major progresses have nevertheless been recently achieved: thanks to wavefront-shaping techniques, or by recording the scattering matrix of a material (its "identity card"), we are now able to force a wave to follow a pre-established trajectory through an opaque medium, and even to image objects through it. Researchers of the GDR COMPLEXE now work to improve the speed of these techniques, to simplify their implementation and to increase their resolution, in particular to make them usable at the industrial level. Imaging directly inside thick complex media remains, in parallel, a major challenge.

MESOSCOPY AND TRANSPORT

The study of wave transport in complex media and of the associated interference phenomena is a core activity of the GDR in a wide variety of areas, such as electron transport in conductors, light propagation in opaque media orthe physics of disordered matter waves. In this context, some phenomena that were so far considered well understood have been recently questioned, such as the very existence of Anderson localization of light. In a similar spirit, in disordered media displaying strong correlations concepts as simple as the one of diffusion seem not to hold any more. Developing a theoretical framework allowing us to understand and to systematically characterize these new systems constitute central challenges for the next few years.

SIMULATING THE QUANTUM WORLD

Exploiting the properties of a wave system to reproduce the physics of the microscopic world has attracted a lot of attention in the past years. Today, the properties of graphene or of topological insulators can thus be simulated by propagating micro-waves or light through properly designed networks. Along the same lines, one can achieve analogues of the mechanism of superfluidity of a quantum gas by means of an optical beam in a nonlinear medium. The GDR supports several research teams working on these questions. There is much to do in the next years, in particular to develop the yet rare experimental setups and to take advantage of the peculiar properties brought by these wave simulators.

GDR ELIOS* NONLINEAR EFFECTS IN OPTICAL FIBERS AND IN INTEGRATED OPTICS

The mission of **Nonlinear effects in optical fibers and in integrated optics (ELIOS)** research network is to bring together the French academic community working on nonlinear effects in waveguides in the broad sense, and to stimulate relations with French manufacturers.

* Effets non-linéaires dans les fibres optiques







10 research topics

Nonlinear effets
iolitons, modulation instability
ogue waves supercontinuum
Parametric processes, Raman and Brillouin processes
elecommunications
iber amplifiers and lasers
hort pulses
Complex dynamics monitoring
Biophotonic applications

PARTNERS CLUB

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Nonlinear fiber optics emerged during the 70's within the context of optical telecommunications. This topic rapidly attracted both physicists to investigate fundamental phenomena and engineers to control light propagation. As an example, physicists immediately identified these waveguides as fantastic testbeds to explore the richness of complex nonlinear effects predicted by the nonlinear Schrödinger equation. From an applicative point of view, optical fibers are extremely versatile and thus extremely useful to optimize the performances of optical sources with various pulse durations at different wavelengths. In that respect, the nonlinear fiber optics community kept moving forward, tailored to other community needs, and took benefit of new opportunities such as the emergence of micro-structured optical fibers or the recent explosion of spatial light telecommunications. In this very competitive international landscape, the French community has always risen and maintained to the top level both in terms of concepts and concrete applications.

Recent top-level publications from the community highlighted the French know-how in the field of nonlinear fiber optics, which stimulated the recent development of innovative techniques to characterize the dynamics of complex nonlinear systems with a high resolution for instance. Meanwhile, nonlinear effects investigation on integrated photonic structures has become a rapidly expanding field of research. On the one hand, the strong confinement of the field inside these waveguides strongly enhances nonlinear effects. On the other hand, these nonlinear waveguides with standard optical functionalities open the way to many prospects to achieve photonic chips suited to different applications ranging from telecommunications, spectroscopy or sensors, to name a few.

These works fall clearly within the context of fundamental studies such as rogue wave formation for instance, or applied ones such as the development of ultra-stable light sources knwon to have a high societal impact. The aim of ELIOS is to create a synergy between different academic actors of the field and to reinforce the link with industrial companies.

GDR EMIE* ISOLATED AND INTERACTING MOLECULAR ASSEMBLIES

The mission of **Isolated and interacting molecular assemblies (EMIE)** research network is to bring together the French community of physicists and chemists working on molecular systems, and covering a wide range of size and complexity. The objects under scrutiny are either isolated in the gas phase or surrounded by a controlled environment. Building upon fundamental aspects of experimental and theoretical molecular physics, our community is naturally inclined to benefit from interactions with other disciplines (chemistry, biology) and to extend its fields of applications to other scientific domains with timely societal impacts (biology, atmosphere).

* Édifices moléculaires isolés et environnés







6 research topics

Experimental methods and instrumentation

Theoretical approaches

Atmospheric and Universe sciences

Excited states and energy

Biomolecules

Environment effects



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PROSPECTS

The main goal of the studies undertaken by EMIE members is to better describe and understand matter at the atomic and molecular scales.

Researchers from the EMIE network contribute to experimental and theoretical methodological developments to characterize molecular assemblies over a wide range of sizes, often by means of frequency- and time-resolved spectroscopic methods.

In the frequency domain, vibrational and electronic spectroscopy are our main source of information on large systems. These skills will be completed in the near future with high-resolution spectroscopy methods, which enable investigating rotational and rovibrational signatures which are particularly robust for studying small and mid-size systems.

We study molecular transformations such as short timescale electronic and nuclear dynamics induced by fast and intense excitations (atto/pico-seconds), and also much slower processes occurring at macroscopic timescales, for instance for slow relaxation mechanisms that can be studied in traps or storage rings.

In terms of spatial environment, our community also covers a wide range of processes, including heterogeneous reactivity, systems that are deposited, solvated or embedded in solid matrices, as well as nanoparticles, with the aim of disentangling the contributions of the environment and of the object itself.

While being structured around fundamental molecular physics and chemistry, our community also explores the application of its specific expertise beyond its own frontiers. In the field of Universe sciences, we contribute to the characterization of molecular assemblies relevant in astrophysics, and to the study of mechanisms involved in atmospheric physics and chemistry. We can apply our expertise to aerosols formation, growth and reactivity, to environment effects, including solid/gas interfaces, and to the formation and evolution of molecular pollutants.

In life sciences, our contribution is based on a strong history of developments in analytical sciences, instrumentation and theoretical approaches, which led the creation of strong connections at the biology-chemistry interface. Studies including environment influence, such as hydration effects on biomolecules, will be further developed in this field too.

In the domain of energy, our studies on excited molecular states can be applied to the dynamics of photoreactive molecules, and we also foresee addressing issues related to the stability of gas hydrates or solvated asphaltenes.

GDR GAZ QUANTIQUES QUANTUM GASES

The **Quantum gases (GAZ QUANTIQUES)** research network gathers this community in a broad sense merging the communities interested in quantum fluids of light and in ultra-cold atoms. These research domains share the same type of scientific questions often originating from condensed-matter physics. They also share a common quantum simulation approach using well controlled and characterized artificial systems. Each experimental system brings complementary advantages. The whole domain is characterized by a strong link between theories and experiments. The GDR will permit discussions and training about both experimental and theoretical novel techniques and will help maintaining the French community at the forefront of research.







Metrology Atom interferometry Quantum gases and fluids Superfluidity Transport Topology Quantum correlations Quantum magnetism Out-of-equilibrium dynamics

9 research topics



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PROSPECTS

Quantum gases are a relatively old subject, starting in 1995 with the observation of Bose-Einstein condensation. Since then, there have been constant progress. In the years 2000s, important results were obtained about superfluid properties, condensates in reduced dimensions, or pair condensation of fermions. In parallel, fountain atomic clocks permit to measure time with an unprecedented precision.

In recent years, the degree of control of ultracold atomic ensembles have continued to progress with important technological advances that have reached the industry. Several companies are involved: Lumibird for the lasers, Thalès and, Muquans for the atomic sensors (clocks, inertial sensors), Pasqal for quantum simulation. In the academic laboratories, technological advances have boosted metrology measurements to even higher precision and accuracy. The best time keeping setups are now optical clocks and more generally atom interferometry allows the measurement of fundamental constants or inertial forces.

These advances permit to realize more complex systems in a yet controlled manner. Ultracold gases have thus become real model quantum simulators owing to their versatility. It is now possible to study situations of interest for condensed-matter problems whose description is challenging for theories and state-of-the-art numerical simulations because of the presence of quantum correlations. We can cite recent results on topological properties with links to graphene physics, on quantum magnetism with the realization of systems with SU(N) symmetry and the condensation of atoms with strong magnetic dipole interactions (chromium, dysprosium), or on out-of-equilibrium physics with the observation of the Kibble-Zurek mechanism... During the last years, quantum fluids of light appeared. In these systems, photons interact in a non-linear medium. Experimental platforms include atomic vapors, photorefractive materials, or polaritons (halfexciton, half-photon particle in planar semiconductor microcavities). Several experiments have for example shown superfluidity effects. One can also structure the medium, leading to an underlying potential. It permits the study of periodic potentials or even simulate topological properties. These artificial systems of light display similar physics as atomic quantum gases and can be described with the same theoretical tools, although with additional twists such as the dissipation linked to absorption which is inherent to photonic systems. Links between the two communities are currently growing and it is natural to merge them into a common GDR to foster mutual fertilization.

RESEARCH GROUP ACTIONS

We will focus on two main annual events: a general meeting and a two-week predoctoral school in Les Houches. The general meeting will aim at maintaining the cooperation and mutual help habits of the community and will favor the emergence of novel research directions and collaborations. The predoctoral school in Les Houches on ultracold atoms is highly recognized, even at the international level. Its themes will now include the fluids of light. It offers students in the field a solid initial training and the building of an international network from the very beginning of their theses. The GDR will possibly also financially support other events (scientific workshops, student scientific meetings, outreach events...).

GDR HoWDI* VAN DER WAALS HETEROSTRUCTURES OF LOW-DIMENSIONALITY MATERIALS

The van der Waals interaction now allows to assemble materials of different nature and dimensionality, 2D (2D materials), 1D (nanotubes, nanowires), 3D (more or less thin films) or 0D (quantum dots, molecules) in the form of heterostructures. Van der Waals heterostructures of low-dimensionality materials (HoWDi) research network brings together teams that explore the elaboration of these heterostructures as well as their novel physical properties, which are inherited from the constituent materials or generated by interface or proximity effects.

* Hétérostructures de van der Waals de matériaux de basse dimensionnalité





4 research topics

Synthesis, nanofabrication, characterization

Electronic transport and its interfaces

Optical and excitonic properties, photonics

Magnetism, spintronics, electronic correlations



300 researchers involved within **90** laboratories

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PROSPECTS

A major evolution in low-dimensional physics arises from the possibility to assemble crystalline materials at the macroscopic scale but with atomic precision, yiel-Controlling the distance between van der Waals mateding 2D, but also 1D and mixed dimensional (2D-1D, rials at the Angström scale as well as the angular degree 2D-0D or 2D-3D) heterostructures. The cohesion of these of freedom (chiral angle in nanotubes, angular mismatch delicate assemblies stems from van der Waals interac-(«twist") between atomic lattices of 2D layers) offer the tions, which led to the now popular name of "van der possibility to truly engineer band structures and to disco-Waals heterostructures". These artificial materials can be ver new electronic and photonic phases or new coupling fabricated at the laboratory scale by inexpensive means, phenomena in the near field. In this context, the emerand have revealed remarkable properties, which have gence of van der Waals materials with a magnetic order had a strong impact in recent years (moiré effects on sumakes it possible to reinvent the physics of magnetic perconductivity and light emission, proximity effects on proximity effects, for example at the interface between the emergence of exotic electronic phases). Our network semiconductor and 2D ferromagnetic materials. addresses theoretical, numerical and experimental aspects associated with van der Waals heterostructures. **METROLOGY AND INNOVATIVE DEVICES**

AN EXTENDED FAMILY

Van der Waals materials have attracted major scientific interest over the past 15 years, first with graphene, then with boron nitride (BN) and later with semiconducting transition metal dichalcogenides. During the last five years, new quantum phases (spin, magnetic and charge order, electronic correlations, electronic and photonic band structure of non-trivial topologies) have been experimentally observed in the 2D limit. Individually, these materials are the subject of dedicated fundamental studies and their integration in van der Waals heterostructures gives access to a multitude of new physical phenomena.

CONTROLLED ELABORATION, CHARACTERIZATION AND MODELING

Increasingly sophisticated «top-down» approaches allow stacking of micrometric sheets by controlling their sequence and relative orientations. These approaches offer almost unlimited possibilities and alongside, access to a whole range of original properties. Albeit conveniently implemented at the laboratory scale, such approaches preclude from obtaining large area, scalable heterostructures. Our GDR aims to promote a national effort on bottom-up approaches in a field where almost everything remains to be done: mastering the quality, crystalline phase and stoichiometry of van der Waals materials, as well as epitaxy relationships and proximity effects within heterostructures. This research is accompanied by advanced characterizations (optical and electronic microscopies and spectroscopies, local probe measurements). These efforts can rely on numerical and modeling efforts to predict the existence and properties of new families of materials and heterostructures.

TWISTRONIC AND PROXIMITY EFFECTS

Van der Waals heterostructures are easily integrated into photonic, electronic, magnetic, mechanical, nanostructures. It is then possible to optimize and control their light emission and/or electronic transport characteristics up to metrological accuracy. More generally, van der Waals heterostructures allow the design of numerous model devices (single photon sources, light-emitting diodes, photodetectors, magnetic tunnel junctions...), whose microscopic operation is controllable by an external parameter (mechanical stress, electric field...). One of the major challenges of this field is to exploit the specificities of van der Waals materials (absence of dangling bonds, lattice mismatch, various electronic and magnetic phases, enhanced Coulomb interactions, valley pseudospin) to obtain new functionalities that cannot be achieved with more conventional materials.

GDR HPERO* HALIDE PEROVSKITES

The **Halide Perovskites (HPERO)** research network is dedicated to halide perovskites. It offers a multidisciplinary approach mixing fundamental and applied aspects, so as to create a synergy capable of developing new concepts as well as opening new potentials in terms of applications.

* Pérovskites Halogénées







6 research topics

Material engineering

Structural studies and defects

Physical properties

Interfaces

Photovoltaics

Emergent developments

175 researchers involved within **42** laboratories (including 4 foreign laboratories)

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PROSPECTS

Hybrid halide perovskites marked a breakthrough for photovoltaics in the early 2010s, with a first record efficiency certified in the NREL diagram at 14.1% in 2013. In 2020, the certified record efficiency reached 25.5%, exceeding those of the thin films or multicrystalline silicon sectors, as well as those of the CIGS one. The use of halide perovskites in tandem solar cells, especially with silicon, should permit to reach soon efficiency records of more than 30% (29.8% reached in 2021 with a silicon / perovskite tandem cell).

These record efficiencies being obtained on small area solar cells, upscaling is an important issue, especially since the solution-processed technologies at ambient temperature of the halide perovskites layers are particularly well suited. Interface engineering has also become a dominant theme in recent years for all photovoltaic sectors (3D, 3D / 2D, quantum dots based solar cells or tandem solar cells on silicon) essentially based on thin films.

Stability problems (of chemical origin or under illumination) of the perovskite solar cells represent a critical issue that has to be overcome. Addressing the stability issue opens several fields of research, with works aiming to (i) understand the underlying mechanisms from both the experimental and theoretical points of view, (ii) develop new interfaces including buffer layers of organic or inorganic materials and search for more relevant hole / electron transporting layers, (iii) tune and optimize the composition of the perovskite layer.

This last topic resulted recently in a renewed interest in layered perovskites, well known since the beginning of the 1990s for their remarkable optical properties. Moreover, low dimensional materials such as nanometric quantum dots and platelets have also emerged as potential avenues of exploration. In turn, the number of perspectives for halide perovskites is growing considerably with:

• a very wide field of exploration for chemical and structural engineering: shaping (crystals, thin films, nanostructures), doping, new cations, lead substitution, encapsulation, interface layers in devices;

• a growing number of applications, some of them are already well underway such as LEDs, laser diodes, detection of ionizing radiations; others are still emergent such as energy storage, thermoelectricity, spintronics/ pinorbitronics, catalysis and photocatalysis (hydrogen production)...

• increasing efforts to understand the physical properties: structural information, nature and role of defects, optical properties (excitons, biexcitons), electronic, spin, transport and mechanical properties, interactions with phonons (polarons), strong anharmonicity of the crystal lattice, physical and chemical mechanisms at interfaces...

The studies carried out within GDR HPERO are based on both experimental and theoretical investigations, largely benefiting from tools and concepts developed for «conventional» semiconductors including the use of major research infrastructures (neutrons, synchrotrons, intense magnetic fields, NMR, GENCI). The concomitant development of new materials, new multiscale spatial and temporal spectroscopies, operando measurements, as well as the increasing complexity of the systems push the GDR teams to take advantage of new theoretical tools such as machine learning.

GDR IAMAT* ARTIFICIAL INTELLIGENCE IN MATERIALS SCIENCE

The mission and main objective of the Artificial intelligence in materials science (IAMAT) research network is to bring together the many teams and different communities interested in artificial intelligence approaches in theoretical and experimental materials science. The scientific topics cover the continuum from AI developments to concrete applications in materials science. The key goals are to promote educational exchanges between communities, particularly through transverse actions, and to foster new inspirations and collaborations.





3 research topics

Machine learning for atomistic and multiscale simulations (quantum models, molecular dynamics, mesoscopic and multiscale modeling)

High-throughput characterization (smarter data collection, accelerated data treatment, data enhancing, feature recognition)

Materials design and structure-properties relations (inverse design, optimization of heterogeneous data, prediction of complex and/or non-measurable properties)



450 researchers involved within **80** laboratories

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MACHINE LEARNING IN SIMULATIONS

The search for innovative materials with optimum structu-Although atomistic calculations have become increaral, thermodynamic, and functional properties is a pursuit singly common tools in materials science, they are inheof mankind. However, the discovery of new efficient materently limited by their computational cost, which limits rials remains challenging. The main approach to this kind the accessible space and time scales. In this context, maof challenge is the identification of structure-property relachine learning methods are and will be used to search tionships and the corresponding design of chemical comfor non-obvious relationships between the atomic strucposition and processing of the optimal material. ture (which can be encoded using a large number of In general, these processing-structure-property-perforpossible descriptors) and the property of interest, inside mance (PSPP) relationships are far from being well unextensive databases. Thanks to the availability of huge derstood. Moreover, the deductive science relationship of amounts of high-quality theoretical data from electronic cause and effect and the inductive engineering relationship structure calculations, molecular dynamics simulations of goal and means tend to proceed along opposite direcand mesoscopic multiscale modeling, machine learning tions. To circumvent this difficulty, different approaches are will provide the French community breakthrough tools developed, including for instance high-throughput screein allowing, through the analysis of the available data, ning, inverse design or genetic algorithms. In this context, the discovery of previously unknown relationships and AI-based approaches, which are more and more used, are the identification of promising new materials. accelerating the pace of discovery of new materials, and have become exceptionally attractive for prediction and de-**HIGH-THROUGHPUT CHARACTERIZATION** sign in many research and application areas.

Over the past decade, advancements in light and particle sources, optics and detector technologies have led to a dramatic increase in the volume and data quality of experimental characterization instruments (diffraction/ scattering, microscopy, tomography, spectroscopy, etc.). These advancements open new perspectives for systematic combinatorial chemistry analysis and in situ and operando ultra-fast and/or spatially-resolved characterizations of materials and devices previously considered technically infeasible. However, these advances come at a cost, related to the handling of the big data collected during these experiments. It is not possible anymore to get real-time feedback regarding the relevance of the data or its quality, and perform on-the-fly adjustments that would allow one to correct the measurement strategy. Artificial intelligence and machine learning algorithms are and will be deployed to address this novel and massive challenge raised by the high data throughput, and allow a much faster and more efficient characterization of new materials.

MATERIALS DESIGN

OBJECTIVES: KNOWLEDGE TRANSFER BETWEEN DIFFERENT COMMUNITIES, TRAINING NEW RESEARCHERS

The primary goals of the GDR IAMAT are twofold: on the one hand, to broaden the community and, on the other hand, to share and transfer, from one scientific community to another, the common expertise and know-how necessary to develop and use new methods to design, model, synthetize, and characterize new materials thanks to AI/ML tools and techniques. The GDR will therefore act as a crossroad of knowledge bringing together various scientific and technical skills that will help promoting new groundbreaking achievements.

The GDR IAMAT also aims at training new researchers in the use of those new techniques and tools, as they will be the first generation of AI-native researchers in materials science. This will help in federating the communities, facilitating interdisciplinary collaborations, and keeping the field up to date with the constantly improving state-of-the-art in research around AI/ML in materials science. We will pay particular attention to attract and train new members - for example, new recruits or people whose subjects could benefit from the use of AI/ ML techniques.

GDR IDE* INTERACTION, DISORDER, ELASTICITY

The mission of the **Interaction, disorder, elasticity (IDE)** research network is to lead to collaborations whose common point is the study of phenomena where heterogeneities play an essential role – both at the theoretical and experimental level – and well described by the framework of disordered elastic systems. The purpose of the GDR is to promote exchanges between communities working on systems of very different nature or scales, although described within this same framework, in order to pool the varied expertise on open questions and initiate new research themes.

* Interaction, désordre, élasticité





6 research topics

Disordered elastic systems

Sheared amorphous materials

Magnetic walls and ferroelectric domains

Growth and propagation of fronts

Plasticity and fracture (avalanches)

Interfaces in biophysics and active matter





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PROSPECTS

CONTEXT

Many physical phenomena are governed by the presence of disorder. Examples range from solid materials (impurities governing fragility and transport), to regular structures such as crystals or foams (where the dynamics is ruled by defects) and to amorphous systems (whose inhomogeneities determine the mechanical behavior). All of these systems have a common property: disorder competes with so-called "elastic" interaction forces, which counterbalance the effects of disorder.

GOALS

The French physics community is at the forefront in the study of such phenomena, at the experimental and theoretical level. This is due to a particular conjunction: the study of soft matter and statistical physics in general are historically highly developed, and a large number of experimental labs in condensed matter and mechanics are very active (both at academic and industrial levels). Through this new GDR, we aim at federating a set of communities that have become partly impermeable to each other.

The topics covered bring together systems as diverse as elastic lines and surfaces driven out of equilibrium, disorder in active matter, structural glasses and complex energy landscapes, or the mechanics of amorphous media. Theoretical and experimental progress in these fields has sometimes taken place in parallel and without mutual knowledge of this progress. We aim at offering ways to remedy this situation, through actions allowing researchers to build bridges between their subjects of interest.

LONG-TERM ACTIONS

Apart from the annual meetings, the GDR aims to support dissemination and animation actions, thanks to the website and to a newsletter. To contribute to a better representation of the field, we support outreach (events, scientific magazines, dissemination of scientific culture), as well as actions carried out at the level of education. One objective is to establish and maintain a thematic bibliography listing reference and review articles, and to set up a dictionary of disordered systems, listing by key words the questions and associated references, the aim being to allow different communities to get along.

INTERNATIONAL

The research conducted in France is carried out in collaboration with teams abroad. A component of the GDR is made up of researchers in Switzerland, in Geneva and in Lausanne, which reflects long-standing partnerships. Other teams in Argentina, Spain, Finland and Italy also have close collaborations on these themes. We want to enable the French community to keep these international links alive and to establish new ones, by conducting a continuous scientific monitoring.

GDR IQFA* QUANTUM ENGINEERING, FROM <u>FUNDAMENTALS TO APPLICATIONS</u>

The mission of **Quantum engineering, from fundamentals to applications (IQFA)** research network is to bring together the French community whose research activities relate to quantum technologies. All quantum information applications are concerned, i.e. communication, processing, simulation, and metrology. Moreover, all quantum information holders are considered, encompassing quantum light, condensed matter, quantum gases, etc., where photons, atoms, electrons, trapped ions, superconductor circuits, etc., play a major role. Also, quantum science and technology applications are investigated regardless of coding strategy, e.g. individual or collective states, and the very nature of the observables.

* Ingénierie quantique, des aspects fondamentaux aux applications





5 research topics

Fundamental quantum science

Quantum communication and cryptography

Quantum computing, hardware and algorithms

Quantum simulation

Quantum metrology and sensors

Transverse engineering and methods





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PROSPECTS

Quantum technologies were born forty years ago from the crossroads between theoretical computing and experimental physics. Progress in the control and manipulation of individual quantum objects now enables to produce more and more complex and functionalized quantum assemblies. Beyond a better understanding of the foundations of quantum physics, these systems can allow the development of secure communications, to execute algorithms faster than conventional computers, to develop ultra-sensitive sensors or even to reproduce physical phenomena inaccessible to direct observations or to classical numerical simulations.

The challenge of the GDR IQFA is to support this booming field of research. Starting from quantum optics and atomic physics, manipulated quantum objects have diversified, with systems from condensed matter physics and fundamental electronics having experienced spectacular progress over the last decade. The number of quantum bits controlled in atomic systems, photons or superconducting circuits has increased from one or two to nearly a hundred, while quantum communications have moved from the scale of a laboratory to that of a country. Understanding and modeling these increasingly complex systems has increased the weight of mathematics, computer science, and control theory of quantum systems. This field has also opened up to chemistry: necessary for the development of quantum materials, it has very recently become a beneficiary of the potential offered by quantum simulations.

A threshold of scientific and technological maturity has also been crossed, making commercial applications sufficiently credible to stimulate the interest of major industrial groups and bring out, via public and private investments, new economic players weaving a network of innovative companies. This new quantum industry fully benefits, for its recruitment, from the skills and versatility of the doctoral students trained in the teams participating in the GDR IQFA, whose strengths are interdisciplinarity and the training of young researchers. The GDR IQFA's mission is to federate around the common language of quantum information researchers from different scientific backgrounds, while maintaining close links between theory and experiment. In a context of very high international competition, both from the academic and industrial worlds, it allows the French scientific community to gather and exchange views annually during the GDR colloquium. This event is an opportunity to cover the entire spectrum of quantum technologies, from questions related to the foundations of quantum mechanics to the development of commercial quantum devices.

It is in the light of these developments that the GDR IQFA, which is entering the last year of its third term, will take stock and prepare its successor, carried by a new team.

GDR ISM* INTERFACIAL SOFT MATTER

The mission of the **Interfacial Soft Matter (ISM)** research network is to emphasize and understand the structure and dynamics of thermally dominated systems near the boundary between a liquid and another phase. ISM provides a forum for the French and international communities - from physics, chemistry and engineering backgrounds and using a diverse set of experimental, theoretical and computational tools - studying the domain to congregate and exchange ideas.

* In english originally





5 research topics

Mechanics of soft interfaces

Surfaces in contact with electrolytes

Active matter

Soft functional layers

Structure-property relations



200 researchers involved within 40 laboratories

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PROSPECTS

The organization and dynamics of soft materials can be deeply altered in the vicinity of an interface since the interaction energies there are typically of the same order of magnitude as those involved in the bulk material. Similarly for the bulk, many soft materials and biological entities can be pictured as "made of interfaces": systems such as suspensions of particles or droplets are formed of mesoscale objects interacting via intermolecular and surface forces, the details of which control the macroscopic material properties.

Interfaces are indeed at the heart of a wealth of challenging problems in today's soft matter science, from DNA transcription, to friction and lubrication, charge regulation, and "smart" functional layers requiring novel syntheses. Additionally, many non-equilibrium systems give rise to spontaneous mobility of particles without the need for an external action. All of these systems, by virtue of their grouping under the heading of "soft", typically bear the signatures of thermal agitation. Combining all of these ingredients, the GDR Interfacial Soft Matter (ISM) was created. The principal themes considered by ISM constitute an emergent field. Those themes concerning mechanics and electrolytes, describing equilibrium as well as structural and dynamical aspects of soft matter, are the most fundamental axes of the ISM domain. These fundamental axes are strongly linked to active matter along with the practical, societal and industrial applications of soft functional layers and the theme of structure-property relations. In this last theme, the questions linked to synthesis and innovative applications of interfacial soft matter are also of great interest to our industrial partners.

GDR LEPICE-HDE* HIGH-ENERGY LASERS AND PLASMAS UNDER EXTREME CONDITIONS

The mission of the **High-energy lasers and plasmas under extreme conditions (LEPICE-HDE)** research network is to bring together the French community working on high energy density (HED) physics related to high energy lasers. Its role is to strenghten the exchange between the numerous research teams with the aim of developing new experimental and diagnostic tools, as well as improving the modelling capabilities for HED physics in the frame of laser-generated plasmas.

*Lasers énergétiques et intenses et plasmas sous conditions extrêmes





6 research topics

Laser-generated shocks, matter under extreme conditions, planetology, geophysics

Hydrodynamics and transport in the context of inertial confinement fusion (ICF)

Laser-plasma interaction: laser beam propagation in warm plasmas, anomalous absorption

Atomic physics in warm and dense plasmas, atomic physics in the presence of intense fields

Laboratory astrophysics in laser plasma experiments

Laser generated radiation sources and their application to high energy density physics and nuclear physics



150 researchers involved within **16** laboratories

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PROSPECTS

The research topics of GDR LEPICE (standing for *Lasers* énergétiques et intenses et plasmas sous conditions extrêmes = high-energy lasers and plasmas under extreme conditions) cover the whole range of high-energy-density (HED) physics that can be accessed with high-energy and high-power lasers, like the physics around inertial confinement fusion (ICF) projects as well as laboratory astrophysics and geophysics.

The research on matter under extreme conditions is of fundamental interest due to its implications with the physics of dense matter, in particular in the context of geophysics and astrophysics. High-energy lasers, such as those developed for the different steps on the way to achieve ICF, as well as laser-generated short-wavelength radiation sources allow nowadays to access and/or to diagnose matter under poorly known conditions of density and temperature. This allows us to advance considerably in our understanding with respect to what has yet been accessible with conventional methods.

The radiation energy that is delivered with the available facilities allows researchers to reproduce in laboratory experiments extreme conditions that are encountered in the Universe (e.g. supernovae, accretion disks, jets, etc.) and, upon that, to realize dynamic studies, impossible to obtain via studies with astronomical techniques.

The studies on plasma hydrodynamics within this GDR are carried out in close coordination between experimental teams and specialists in theoretical-numerical modelling. The results obtained from French and international laser facilities, together with the modelling, provide major advances in the understanding of the dynamics of plasmas under extreme conditions.

The research on laser-plasma interaction presents a key activity in the frame of the GDR for the physics of laser fusion, for the laser-plasma coupling of ultrahigh intensity (UHI) lasers, as well as for generation of secondary radiation sources. The complementary competences unified in this GDR allow us to advance in the understanding and modelling of propagation, absorption, diffusion, and pulse amplification of intense coherent light beams in plasmas.

Secondary radiation sources due to laser-driven collective electron motion have an important potential of application in HED physics. Proton- and electron beams generated via UHI lasers, nowadays available on every major laser facility, are extremely important elements in HED experiments, in particular for diagnostic purposes.

Atomic physics in dense plasmas plays an important role for several of the research axes of this GDR, in particular for radiative transport in plasma hydrodynamics. Studies on opacities of strongly correlated plasmas play an important role in ICF and astrophysical plasmas for the understanding of hydrodynamic (Rayleigh-Taylor) instabilities and of radiative shocks.

The activities on laser-driven nuclear excitation within this GDR are at the interfaces between nuclear and atomic physics, as well as the physics of warm plasmas. These very innovative studies have the goal to explore the modifications on nuclear states by external (laser) fields in ionized matter.

Several recent UHI laser facilities, now accessible in France (Cilex-Apollon) and in Europe (ELI), will soon give access to laser intensities that can expose the vacuum and matter (plasmas!) to extreme electromagnetic fields. By successively increasing the field strength by improving the performance of such lasers, it will be more and more likely to provoke phenomena of quantum electrodynamics (QED), e.g. e^-e^+ pair production, that have not yet been observed with other facilities (colliders etc.). Several groups within the GDR have started studies to explore the way to access this exciting QED regime with the actual and forthcoming conditions of laser facilities.

GDR MECAQ* QUANTUM OPTOMECHANICS AND NANOMECHANICS

The mission of the **Quantum optomechanics and nanomechanics (MecaQ)** research network is to bring is to bring together the French research community in the fields of nanoechanics and optomechanics, in particular in the regime where quantum fluctuations matter. Metrology, ultrasensitive measurements and quantum information are among the research topics covered by GDR MecaQ.

* Optomécanique et nanomécanique quantiques







Nanomechanics and nonlinear optics Theory of nanomechanical systems Optomechanical sensors Quantum optomechanics Hybrid systems Optomechanics and fundamental physics Electro-optomechanics Nano-fabrication & nanomechanical engineering Micro-/nano-optomechanics in industry Nanophononics and phonon transport 120 researchers involved

11 research topics

Quantum thermodynamics



PARTNERS CLUB

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PROSPECTS

An important research topic of the 2010's decade has been "quantum" mechanical systems, mechanical resonators so sensitive that a full description of their dynamics requires a quantum treatment. The GDR Quantum optomechanics and nanomechanics fosters research activities on these topics, related to quantum measurement and control, with new stakes and very ambitious challenges.

TECHNOLOGICAL STAKES AND CHALLENGES

The main technological stakes in developing quantum mechanical systems are similar to those encountered in emerging quantum technologies, with the recent perspective of a new generation of ultrasensitive sensors and communication systems, possibly embedded in compact packages for wide applications. To name a few, development of coherent opto-electromechanical transducers between the optical and the microwave bands, hybrid mechanical systems (where a mechanical degree of freedom is strongly coupled to another quantum system), nanooptomechanical crystals (possibly used as topological insulators), nanooptomechanical probes, definition of new metrological standards, etc. The associated technological challenges are related to the effects of decoherence, which have to be strongly minimized. Tremendous progress have been recently performed in this direction, with nanomechanical systems with quality factors above one billion at room temperature. Designing fabrication processes that allow simultaneously very low optical and mechanical losses however remains a huge technical challenge, that still requires an important research effort.

FUNDAMENTAL STAKES AND CHALLENGES

Technological progress in ultrasensitive mechanical systems are also motivated by fundamental physics issues, in what is commonly called the second quantum revolution. These include demonstration of displacement measurement experiments at or below fundamental sensitivity limits, macroscopic demonstration of mechanical energy quantization, back-action evading measurements, creation of non-classical mechanical states, or the impact of gravitation on the decoherence of macroscopic systems. These issues are at the heart of an important research effort to understand their impact at the macroscopic scale and to design measurement protocols that lower or evade quantum bounds.

GDR MEETICC* UNCONVENTIONAL MATERIALS, ELECTRONIC STATES, INTERACTIONS AND COUPLINGS

The mission of the research network **Materials, electronic states, interactions and unconventional couplings (MEETICC)** is to bring together the French community of experimental and theoretical scientists, chemists and physicists, who study materials with unconventional electronic states and couplings. Once under control, the remarkable properties of systems such as multiferroics or topological insulators could lead to breakthroughs in the fields of energy and information technology.

*Matériaux, états électroniques, interactions et couplages non-conventionnels





3 research topics

Remarkable properties in highly correlated systems (magnetism, superconductivity)

Unconventional electronic states in topological phases and confined systems

Unconventional electronic materials and properties





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PROSPECTS

The scientific prospects of the GDR MEETICC are presented according to its three axes of research.

AXIS "HIGH-CORRELATION SYSTEMS"

Recent advances involve chiral interactions (Dzyaloshinskii-Moriya), at the origin of original magnetic mesostructures (skyrmions, hopfions). As far as superconductivity is concerned, a strong activity is developing around pnictides, chalcogenides and iron silicides (discovered in France). The understanding of their phase diagram, mixing exotic phases and unconventional superconductivity, could allow the identification of superconductivity mechanisms. Note the emergence of themes related to electronic surface states, out of equilibrium, or associating electronic correlations and spin-orbit coupling as in iridates.

AXIS "UNCONVENTIONAL ELECTRONIC STATES OF TOPOLOGICAL PHASES"

We foresee developments concerning the topological properties of correlated systems (Mott insulators; heavy fermion superconductivity), or Weyl semimetals. Moreover, 2D metallic or even superconducting electron gases open the way to emerging electronics and topologically protected quantum computing (Majorana quasiparticles).

AXIS "EMERGING MATERIALS"

We can note the development of oxyhydrides inducing atypical valence states (Ni⁺, Ru²⁺, etc.) that can lead to new phases, and the global prediction of topological properties, based on space group and band theory. Finally, the control of properties at interfaces – such as multiferrocity, spin/charge current conversion - is strongly emerging and could lead to new heterostructures, associating topological insulators or ferromagnetism with novel physical properties.

Our research will benefit from impressive advances in experimental techniques using extreme conditions of pressure, temperature and electric/magnetic field, giving access to unexplored regions of phase diagrams. Let us underline the considerable development of ultrafast techniques (femtosecond or even attosecond; european XFEL sources, HHD sources, etc.), giving access to new exotic out-of-equilibrium states and allowing the decoupling of interactions simultaneously at work in our systems.

GDR MESO* **MESOSCOPIC OUANTUM PHYSICS**

The mission of the Mesoscopic quantum physics (MESO) research network is to bring together the French community whose activities are focused on coherent electronic transport in conductors of all sizes and types (hybrid systems, topological insulators, graphene, etc.). Recent theoretical and experimental developments focus on the manipulation of the quantum states of such systems, and on very large bandwidth experiments.

*Physique quantique mésoscopique





Coherent manipulation of charge and spin degrees of freedom

Hybrid systems, Dirac and topological matter

Open quantum systems

Mesoscopic thermodynamics





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PROSPECTS

WHAT IS AT STAKE?

The general theme of the GDR MESO is the study of the coherent manipulation of charge and spin degrees quantum properties of conductors, mainly through transport measurements that provide information on of freedom; hybrid systems, Dirac and topological matter; the wave nature of the charge carriers, but also through open quantum systems; current noise measurements that provide information ٠ mesoscopic thermodynamics. on the corpuscular nature and thus the statistics of the carriers. Recent years have seen the emergence New theoretical and experimental means allow probing of local probe techniques (capacitive measurements, systems in limits never explored before, beyond the tunnel transport measurements, etc.), finite frequency simple perturbative approach. One of the challenges of measurements (to reach the regime where the excitation our GDR is to promote a scientific culture that allows us frequency is comparable to the characteristic frequencies to approach quantum systems with a transversal vision, of the circuit) and hybrid experiments combining optics combining approaches from other communities. and transport. Most of the experiments are performed at low energies (below 100 µ eV and at very low temperature **CHALLENGES** 10-100 mK).

The GDR remains very focused on fundamental "physics", even if we keep potential applications in mind. In particular, our work can have direct impacts on quantum information science. Indeed, if the miniaturization of electronic components continues, the electronics of the future could enter fields where quantum effects play an important role. All research on quantum bits justified by the prospect of a possible quantum computer has led to the understanding of many underlying mechanisms responsible for the loss of quantum coherence. Another very important point is the emergence of new types of materials or topological matter. Graphene is an obvious example where advances in the fabrication of high mobility samples have made it possible to realize resistance standards for metrology based on the quantum Hall effect that do not require liquid helium cooling.

The fundamental challenges are divided into 4 axes :

The systems we study naturally contain many interacting particles. Thus, one of the challenges is to solve the N-body problem, regardless of the type of Hamiltonian, time-dependent or not. This challenge is both theoretical and experimental, since to deal with such problems, new theoretical tools must be combined with experiments to probe ever more complex quantities.

GDR NANOPERANDO* STRUCTURE AND DYNAMICS OF MATERIALS IN REAL ENVIRONMENTS

The mission of the Structure and dynamics of materials in real environments (NANOPERANDO) research network is to bring together the French community studying the structural dynamics of materials in their formation or application media. Although in situ or in operando analysis have been developed on all the techniques that allow investigating matter at the atomic scale, it remains nevertheless a very young science and its future progress requires the emergence of interdisciplinary synergies that could open new fields of research in material sciences, but also in Earth and life sciences.

* Structure et dynamique des matériaux dans leur environnement « réel »





5 research topics

Synthesis and self-assembling of nanomaterials

Reactivity of nanocatalysts

Electrochemical reactions

Structure and dynamics of biomaterials in their native environments

Life cycle of (nano)materials in natural and biological media





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PROSPECTS

Here are the goals of the actions and events organized by the GDR Nanoperando:

Stimulating collaborations between experimentalists (developers) of environmental techniques and potential users specialized in materials, by confronting the current possibilities and limits of environmental analysis techniques with the needs of users.

Bringing together three communities of experimentalists (electron microscopy, near-field microscopy and synchrotron techniques), which despite their common goals, strategies and problems still collaborate too little. This diversity of technical skills within the GDR will be an essential asset to effectively cover its thematic plurality.

Exploiting the complementarity of environmental techniques and initiate the development of correlative multi-scale approaches. Confronting the results obtained with different techniques will allow a better understanding of the *in situ* phenomena under study and the artifacts inherent to each technique (electron beam effects, tip effects, interpretation of synchrotron data, etc.). This approach will also facilitate the transfer of ideas and even technologies between techniques. It is also important to establish common data acquisition and processing protocols, including machine learning approaches that can be applied to different techniques and experiments.

Identifying and removing the technical barriers preventing the use of environmental techniques on certain types of samples. Given the diversity and complexity of observable phenomena, it is essential to set up interdisciplinary working groups that are aware of the instrumental constraints and specific requirements related to the nature of the samples and their environment.

Coupling experience and theory. In parallel with the recent progress of *in situ* analysis, theoretical approaches are being developed to understand the thermodynamic properties of nanomaterials in interaction with their environment. By bringing together experimentalists and theoreticians, the GDR will generate new synergies and establish a unique pole of expertise that is essential for quantitatively interpreting dynamic and complex phenomena.

GDR NS-CPU* NANOSCIENCES WITH NEAR-FIELD MICROS-COPY UNDER ULTRA-HIGH VACUUM

The mission of the **Nanosciences with near-field microscopy under ultra-high vacuum (NS-CPU)** research network is to bring together the French community whose "nanoscience" research activities are based on scanning probe microscopy (SPM) techniques operating under ultra-high vacuum (UHV). Indeed, a typical phenomenon in nanoscience results from a physical, chemical, magnetic, mechanical or optical fact that must be measured by individual and direct observations with spatial precision of the order of a picometre.

* Nanosciences en champ proche sous ultra vide





5 research topics

Electronic and vibrational structure of individual nanostructures and nano-objects

Nanometer-scale light-matter interactions

Study of local magnetism and quantum states

Electronic, electrostatic properties and charge transfer

Theoretical concepts and computational tools



125 researchers involved within **20** laboratories

PARTNERS CLUB

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PROSPECTS

Backed by surface science, nanosciences intersect many scientific and technical research fields: nanoelectronics, molecular electronics and mechanics, nanomagnetism, the physics of semiconductors and superconductors, the physics and chemistry of individual nano-objects, heterogeneous catalysis, metallurgy, etc. The techniques of choice for the study of nanosciences are near-field microscopy techniques (STM, STM-photon, STM + magnetic field, STS, NC-AFM, KPFM), which work under ultrahigh vacuum (UHV) and at different temperatures (e.g., at 4 K, 77 K and 300 K). They provide direct access to the topography of the surface but also to the electronic, optical or magnetic properties of a single nano-object, a molecule, an atom or a surface state.

ELECTRONIC AND VIBRATIONAL STRUCTURE

Scannig tunneling spectroscopy (STS) provides access to the electronic structure of matter down to the atomic scale through I(V), I(Z) and differential conductance measurements. This technique allows measuring the electronic spectrum of individual nano-objects (a molecule, a nanostructure), and also probing the electronic properties of low-dimensional materials (nanotubes, graphene and other two-dimensional materials). Vibrational states can be probed by inelastic spectroscopy both on an individual nano-object and on nanomaterials.

LIGHT-MATTER INTERACTIONS

The optical properties of a single nano-object, such as a quantum dot, a fluorescent molecule or an atom, critically depend on their interactions with their nearby environment (<10 nm). Various mechanisms such as a transfer of charge or energy between the tip and the nano-object can be used to probe, modify or exacerbate the properties of these nano-objects. Experiments combining, under ultra-vacuum, tunneling and optical microscopies, allow direct observation of these mechanisms. The development of approaches combining STM and pulsed lasers opens a path towards pump-probe experiments combining atomic-scale spatial resolution and femtosecond time resolution.

LOCAL MAGNETISM AND QUANTUM STATES

The study of the electronic properties of bulk materials, low-dimensional materials or individual nano-objects presenting a non-trivial quantum state (magnetic, superconducting, charge or spin-density-wave, Mott insulator, topological insulator or topological superconductor, etc.) has grown significantly with the development of (very) low temperature UHV STM techniques, including those ones coupled to an external magnetic field. These techniques enable observing the quantum order parameters, the charge or spin local orders at the atomic scale. Recent instrumental developments aim at probing time-resolved and/or frequency-resolved (up to few dozens of GHz) elementary electronic excitations.

ELECTROSTATIC AND CHARGE TRANSFER

Electrostatic phenomena at the elementary charge scale can be observed in non-contact atomic force microscopy (nc-AFM) coupled with Kelvin probe microscopy (KPFM). The techniques measure the topography with nanometer or even atomic resolution (nc-AFM) and the surface potential (KPFM), which is linked to electrostatic (dipoles, charges) and electronic properties (work function, doping, etc.) of the surface and of a single nano-object (a nanoparticle, a nano-island, a molecule, an atom, surface defects, etc.).

THEORETICAL CONCEPTS AND COMPUTATIONAL TOOLS

The description of the "tip-surface" interactions (with or without a supported nano-object) such as the exchange, electrostatic, van der Waals and magnetic interaction is the basis of all calculations making it possible to predict and reproduce the following different experiments that can be carried out in the near field: topography imaging experiments (STM, NC-AFM), d^n/dV^n , dl/dZ and dZ/dV spectroscopy (STS) in STM, $\Delta f(Z)$ and $\Delta f(V)$ spectroscopy in NC-AFM as well as atomic or molecular manipulation experiments. The interpretation of the experimental data will support the development and provision of calculation codes based on the quantum and/or semi-classical description of these interactions.

GDR OR-NANO* NANOSCALE GOLD AND GOLD NANOPARTICLES

The mission of the **Nanoscale gold and gold nanoparticles (Or-nano)** research group is to initiate and support collaborations of its researchers on topics related to gold nanoparticles, nanoscale gold films or gold-based complexes. The GDR organises two series of regular events in France: the Or-nano conferences which are of multidisciplinary nature and the Or-nano Discussions which aim to deal in depth with a hot topic. Particular support is offered to doctoral students, notably through exchange grants between affiliated labs to participate in scientific events. Or-nano strongly encourages its members to carry out outreach activities in order to make the general public aware of the research conducted in its laboratories. Since its creation in 2006, Or-nano has confirmed its dynamism by regularly evolving its topics, and thus aims to actively contribute to the relevance of French research on the world stage.

* L'or nanométrique et nanoparticules d'or







9 research topics

Plasmonic nanostructures, nano-antennas, modelling

Hot electron physics and plasmonic catalysis

Nanoparticles for nanoelectronics and molecular electronics

Reactivities at interfaces: biosensors, life diagnosis and electrocatalysis

Synthesis of gold nanoparticles and nanoparticle assemblies with controlled morphology

New instrumental challenges for the characterization of single nano-objects: optical microscopies, X-ray microscopies, synchrotron facilities

Fluorescence and magnetic properties of gold complexes and gold clusters

Gold nanoparticles for health: toxicity, delivery, theranostics, clinical applications

Transverse axis: gold in the history of science, in the science-society dialogue and in heritage objects



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PROSPECTS

The topical positioning of the GDR Or-Nano is particular because of the very specific status of gold nanoparticles, which fall within various disciplinary fields such as fundamental nanophotonics, plasmonics, reactivity, biochemical functionalization, new chemical synthesis processes, advanced therapies, numerical simulations, etc. Many emerging themes lie at the crossroads of these disciplines.

HOT ELECTRON PHYSICS

Hot electrons are electrons that are strongly excited above the Fermi level: either via an STM, or by an optical wave or electron beams. They correspond to excited states with a finite lifetime, of the order of a few tens of femtoseconds. Plasmonics is a way of amplifying the effect of hot electrons and opens up a new field of physics where optics and condensed matter physics are combined. Hybrid nano-systems (metal/semiconductor) involving gold nanoparticles are also of great interest at the present time, particularly for understanding the exaltation of chemical reactivity in the vicinity of these nano-systems in heterogeneous catalysis.

PLASMONICS, NANOTHERMICS AND QUANTUM PLASMONICS

Plasmonics makes it possible to manipulate the optical near field by playing on antenna effects and to concentrate the field on dimensions well below the wavelength. Gold nanoparticles are also increasingly used as optically controllable heat nanosources. In particular, they allow the study of thermal phenomena on small scales. Quantum plasmonics is largely a continuation of the work carried out to date in non-linear plasmonics, but it allows us to envisage relatively integrated quantum optics in the long term. From the point of view of classical nonlinear plasmonics, efforts are focused on multipolar nonlinear optics and its applications, particularly for sensing.

TOWARDS CLINICAL APPLICATIONS OF GOLD NANOPARTICLES

Unlike ionic gold, which has been used for decades in medicine and has the benefit of more than 70 years of hindsight, gold nanoparticles in health remain a cutting-edge subject whose work and trials, although constantly increasing, are only just beginning to reach the clinical development stage. The hindsight and expertise gained in recent years by the Or-nano scientific community now allows it to turn to resolutely interdisciplinary and translational research in order to address issues of clinical interest.

GDR P&O* POLYMERS AND OCEANS

The mission of the **Polymers and Oceans (P&O)** research network is to bring together the French community working on the future of plastics in aquatic environments with the aim of promoting the emergence of new interdisciplinary research on this subject. The major asset of the GDR P&O is to mobilize all the scientific communities concerned: chemists, physicists, biologists, ecologists, ecotoxicologists, oceanographers, economists and sociologists in order to support the development of multi-scale and transdisciplinary approaches.

* Polymères et Océans





3 research topics

Plastics: from their entry into the environment to their ultimate fate

Impacts of plastics and long-term risks

The tracks for the future



240 researchers involved within **50** laboratories

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PROSPECTS

PLASTICS: FROM THEIR ENTRY INTO THE ENVIRONMENT TO THEIR ULTIMATE FATE

What are the quantities contributed by each of the sources of contamination (rivers, coasts, sea), what is the true level of contamination of the oceans (surface, water column, seabed, sediment) and how to model the plastic cycle taking into account the land-sea continuum to the abyss? New scientific protocols must be developed to take into account all scales ranging from macro-, to micro and nano-plastics. Much fundamental knowledge about the behavior and ultimate fate of plastics in the environment remains to be acquired. In order to assess the degradation times of polymers in a medium as complex as the environment, it is more than ever necessary to understand the links between their structural and/or morphological properties and their (bio) degradation and fragmentation processes.

IMPACTS OF PLASTICS AND LONG-TERM RISKS

What are the impacts of the accumulation of plastics in theaquatic environment on organisms and the functioning of ecosystems? How do micro- and nano-plastics and associated contaminants interact with cell envelopes and what are their transfer capacities within tissues and cells? The toxicity of microplastics is that they consist of a complex and dynamic mixture of polymers and additives, to which organic matter as well as chemical and biological contaminants can additionally bind. The mechanisms of colonization and biofilm formation, the role of plastics in the vectorization of species, the biodegradability of polymers are all topics that need to be deepened. Taking into account the great diversity of plastics and the complexity of the natural environment,

laboratory research must also acquire an ecosystem



dimension.

THE TRACKS FOR THE FUTURE

What are the preferred solutions for the future? How can an interdisciplinary scientific community respond to this societal, environmental, economic and political demand? In the years to come, it is necessary to be able to offer alternative innovative polymers, whose biodegradability can be controlled by playing on their physico-chemistry, and whose future and potential impacts at the end of their life will be anticipated at the stage of their design. To take into account the social and economic dimension of the problem of plastic pollution in the oceans, questions pertaining to the implementation of new economic models and the perception of environmental issues by society will also be raised.

GDR REST* THEORETICAL SPECTROSCOPY MEETINGS

The mission of the **Theoretical spectroscopy meetings (REST)** research network is to bring together the French communities of theoreticians and numerical simulators of electronic excited states. The objective for the researchers is to exchange and compare with a twofold objective (and common denominator): i) to develop "new" theory for electronic excited states; ii) to model real materials (bulk, surfaces, molecules and nanostructures) with a strong technological interest.

* Rencontres de spectroscopie théorique





6 research topics

Fundamental development: going beyond perturbation theory

From screening to spectroscopy

Effective approaches for a wide range of spectroscopies

Quantum chemistry and solid state physics

Valence and core excitations

Strong vs weak correlation



150 researchers involved within **52** laboratories

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REAL-TIME AND BEYOND EQUILIBRIUM

The development of real-time techniques (as opposed to linear response frequency domain), especially in the framework of Green's function and density functional polarization theories was one of the major recent outcomes of the electronic excitations community. Members of the GDR REST have also been involved in these important developments, and are strongly contributing in explaining recent exciting experiments, going much beyond previous theoretical approaches.

BEYOND PERTURBATIVE APPROACHES

Perturbative approaches (like the GW approximations or the linear response TDDFT) have been very successful in describing photoemission spectroscopy or electron energy loss spectra. Today's developments however permit to go beyond the first order perturbation theory (being first order in the external potential, or in the screening, etc.), so to tackle more complicate systems (strongly correlated) or new features (like double plasmons, or satellites in photoemission). The researchers of our network greatly benefited from the gathering action Strong versus weak correlation. So a completely new scenario opens in the domain of electronic excitations, that require profound theoretical investigation, at the fundamental level ("how to solve an integro-differential equation, without going towards perturbation theory or Dyson equations?", for instance). The REST community is deeply involved in this new strategy.

TOWARDS NEW SPECTROSCOPIES

The development of the *ab initio* screening beyond dipole approximation and with the inclusion of excitonic effects opened the way to new features (excitonic satellites in photoemission), to new spectroscopies (coherent inelastic X-ray scattering, resonant inelastic X-ray scattering, X-ray absorption beyond dipole approximation, etc.) and to new ideas (like Bose-Einstein condensation of excitons) to be exploited in the near future by the REST community.

NEW CHALLENGES FROM EXPERIMENTS

The last four years have witnessed an enormous progress and new directions and investments are being made as we write. New directions, strategies and investments strongly influence the development of theory.

The interaction between matter and strong laser fields has been extensively studied in the last decades, particularly in atoms and molecules. This is however not the case for a crystal. Up to very recently, it was not possible to let a solid interact with a strong laser field (in order to generate higher harmonics, for instance) without destroying the sample. It was only in 2011, in fact, that it was shown the high harmonic generation in a solid of ZnO, opening completely new possibilities, in particular for what are considered table-top synchrotrons. This exciting field needs to be tackled from many sides, for the solid-strong laser field interaction involves many degrees of freedom (surface effects, lattice-electron interactions, quantum nature of photons) and requires a community rather than a group to be efficient.

The need of the theoretical counterpart to new and more challenging experiments will soon have a new meaning, with a new generation of synchrotrons that are seeing the light all over the world. Many among important synchrotrons in fact have shut down for upgrade. The objective is to acquire unprecedented resolution, coherence and, by consequence, the capability to carry out new and exciting discoveries and analyses.

GDR THÉORIE & CLIMAT* THEORETICAL CHALLENGES FOR CLIMATE SCIENCES

The Theoretical Challenges for Climate Sciences (Théorie & Climat) gathers the community of theoreticians: physicists, climatologists, oceanographers, atmospheric scientists, mathematicians, computer scientists, numerical scientists, machine learners, who work on climate sciences. Its aim is to develop innovative theoretical and numerical tools to overcome current scientific gaps. Approaches in statistical physics, turbulence modelling, mathematics and machine learning will help to deepen the understanding of fundamental mechanisms, improve models, and better predict extreme climate events to reduce uncertainties about the impacts of climate changes. This GDR has a strong interdisciplinary vocation and involves researchers from several CNRS institutes, many other French scientific organizations, and private companies.

*Défis théoriques pour les sciences du climat







10 research topics

Climate dynamics

Ocean and atmospheric dynamics

Machine learning and climate

Mathematics and climate - Statistics

Mathematics and climate - Numerical analysis and data assimilation

Stochastic modelling

Physics, non-linear dynamics and climate

Statistical physics and climate

Turbulence and geophysical flows

Relationship between observations, data and model integration



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Understanding and modelling the dynamics of climate This specific example of climate sensitivity illustrates the and its main components, such as the atmosphere, the ocean, the biosphere, or the cryosphere, are major need to develop new theoretical, numerical, and mathechallenges. Indeed, they have major influences on humatical tools to complement traditional approaches. The GDR will address a range of such challenges, for example: mans and their societies, on non-human life forms, and on Nature as a whole. Understanding these dynamics and their future evolution is also an imperative for the How to integrate data and theoretical constraints, safeguard of our civilization, necessary for the characteusing machine learning approaches, to build new generations of climate models? rization of the political issues related to climate changes and for the scientific analysis of its solutions, through How to reduce uncertainties in climate sensitivity the management of risks and a better understanding of estimation? How to reconcile machine learning approaches with the physical constraints allowing for harmonious development. These dynamics are also directly linked to key traditional scientific approaches? technologies and industries, such as weather prediction, • How to reduce uncertainties in the estimation of the probabilities of extreme events? energy, and insurance.

However, it is often forgotten that understanding these complex dynamics is also a set of basic science issues. Indeed, most of the key questions in these fields cannot be answered accurately and satisfactorily using current scientific tools. For example, climate sensitivity, that is the temperature increase when doubling the CO₂ level in the atmosphere, is estimated by the latest IPCC report (AR5) to be between 1.5 K and 4.5 K, with a probability of 0.66. Global warming thus appears clear and scientifically indisputable, at the qualitative level. However, we can see that its quantitative estimate is marred by significant uncertainties.

This lack of precision has major implications for the analysis of global issues. The current state of science is unsatisfactory despite remarkable progress in recent decades. In the specific case of climate sensitivity, going beyond this to a more quantitative science requires fundamental advances in cloud dynamics, boundary layer turbulence and the integration of effective models into climate models. These fundamental advances do not seem to be accessible with traditional approaches. Instead, an approach combining observations, stochastic process modelling and machine learning tools that integrate the dynamics aspect could help to solve this challenge.

- How to make quantitative the study of past and potential future climates?
- How to build effective models whose limits are rigorously quantified?

GDR UP* ULTRAFAST PHENOMENA

The **Ultrafast Phenomena (UP)** research network is dedicated to the study of all phases of matter (gas phase, solid, nanometric, liquid and plasma) at ultrafast timescales (attosecond, femtosecond and picosecond). The French community of ultrafast science is very strong and particularly recognized at the international level. This is due to its high-level experimental and theoretical capabilities, as well as highly recognized laser companies. This research field is strongly expanding because of the development of new laser technologies (at the laboratory scale or at large scale facilities such as FEL or ELI) and computational capabilities, which allows addressing new questions, from the most fundamental (quantum coherence) to applications (optimization of smart materials). The mission of the GDR UP is to stimulate the structuration of our community and to provide an analysis of the state-of-the-art and prospects of our research field.

* In english originally







7 research topics

Attosecond science

Secondary sources of electrons, photons and protons

Dynamics in gas phase atoms and molecules

Femtochemistry-femtobiology

Dynamics in materials and nanostructures

Instrumentation and data

Communication



PARTNERS CLUB

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livering XUV and X-ray femto (fs) or attosecond (as) intense pulses is an important opportunity for the French ultrafast community. Additionally, compact and highly performing laboratory scale light sources are under development. They allow performing complex and time consuming experiments. This includes fs particle sources (electrons, protons) for applications in imaging, or X-ray fs, to study warm and dense matter. High repetition rate (kHz et MHz) sources are able to explore a broad range of wavelength from X to THz (broad band or intense sources). UV-X as pulse generation with highly precise control of the duration and spectrum will allow the study

(kHz et MHz) sources are able to explore a broad range of wavelength from X to THz (broad band or intense sources). UV-X as pulse generation with highly precise control of the duration and spectrum will allow the study of electron dynamics with Angström accuracy. Controlling the light polarization state (orbital angular momentum) is also a crucial undergoing development with direct applications to study symmetry and magnetic properties of matter.

PROSPECTS

FACILITIES ... TO COMPACT SOURCES

EXTREME LIGHT SOURCES: FROM LARGE SCALE

The emerging large scale laser facilities (FEL or ELI) de-

ACCESS TO ULTIMATE TIME SCALE: ATTOSECOND SCIENCE

France is one of the pioneering and leading country in attosecond science. One of the current goal is to be able to study small quantum systems (atoms, small molecules) to measure coherence and guantum states, which requires the development of « complete » experiments, able to access all anisotropies. The field also evolved towards the study of complex molecules (attochemistry...).addressing the question of the reactivity of molecules of biological, chemical or astrochemical interest. The possibility to study molecular ions is emerging. Experiments performed with condensed matter are under development with specific interest to study topological, correlated, magnetic or 2D materials. New approaches such as transient absorption, angularly resolved photoemission, coincidence, spin resolution are now proposed. With the increasing complexity of the experiments, new ad-hoc theoretical developments and strong links between theoreticians and experimentalists becomes compulsory. This includes the description of non-adiabatic electron-nuclear dynamics, correlation and non-linear processes.

MULTISCALE APPROACH IN PHOTOCHEMISTRY AND PHOTOBIOLOGY

The goal is to understand photoactive molecular structures with increasing complexity (from organic molecules to proteins, or supramolecular assemblies) in relation with biological processes, photocatalysis or chemical energy conversion. Highly performing new spectroscopic methods using large spectral and temporal range are currently being developed (ex: 2D UV-visible and IR spectroscopy, UV-visible fs and ps circular dichroism). They allow resolving and understanding complex structural transformations or energy and charge transport at the atomic scale. An accurate understanding of the reactivity requires theoretical developments, with a strong link with experiments. Theoretical approaches are developed to understand molecular reactivity induced by ultrafast ionizing radiation (light or electrons) in relation with radiolysis and radiative damage.

PROBING THE DYNAMICS OF ALL (QUASI-) PARTICLES IN COMPLEX MATERIALS

The joint use of traditional optical femtosecond, THz and pulsed X-ray source opens the way to study out-of-equilibrium processes in new materials showing ultrafast dynamics involving electrons, spins and phonons. Femtosecond time-resolved ARPES allows studying 2D materials (e.g. dichalcogenide transition metals) or Weyl topological semi-metals. Transient absorption at the fs timescale allows to study excitons (e.g. in layered material such as perovskites). New experiments aiming to access spin dynamics, including spin currents or spinto-charge conversion are being developed. New approaches combining electron microscopy and ultrafast radiation emerge. Measurements correlating optical and structural properties with nanometric resolution are becoming possible, by combining cathodoluminescence and microscopy (applied to nano-diamonds and InGaN quantum wells).

GDR XFEL* SCIENCE WITH XFELS

The mission of **Science with XFELs (XFELs)** research network is to bring the French community of involved researchers in studies using X-ray free-electron lasers (FELs) emitting in the X-ray domain. At the interface of physics, chemistry and biology, the XFEL GDR aims at sharing know-how and at maintaining the community aware on the fast evolution of the possibilities provided by this kind of installation.

* Science avec les XFEL





5 research topics

Condensed matter physics

Atoms and molecules in diluted samples

High-energy density

Photochemistry

Structural biology





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PROSPECTS

XFELs are large facilities producing ultrashort light pulses (UV or X) characterized by a brilliance 9 orders of magnitude higher than 4th generation synchrotron facilities. This kind of installations are running in Germany, United States, Japan, Italy, Switzerland, South-Korea and soon in China. The short pulse duration (5-100 fs), the intensity (10¹⁰-10¹² photon/pulse) and the pulse focus dimension (0.1-20 μ m), combined with the extended X-ray energy range (from XUV to hard X-rays) allow to perform innovative experiments not feasible with other types of light sources. The involved scientific topics are condensed matter physics, geoscience, laboratory astrophysics, plasmas, photochemistry, atomic and molecular physics and structural biology. Unique characteristics of light pulses allow, in each domain, to perform time-resolved experiments and to study ultrafast dynamics.

We observe a growing number of members of the french XFEL users' community, with international projects lead by CNRS, CEA and universities. The XFEL community is specific because it brings together – and sometime a beamtime – physicists, chemists, geoscientists, astrophysicists, materials engineers and biologists, all motivated by conducting experiments at the limits of feasibility in order to answer questions unsolved so far.

Although the scientific topics are diverse, experimental bottlenecks are often similar, explaining the development of common culture, founded on scientific exchange on the data acquisition or data treatment. The first goal of the XFEL GDR is to create a privileged space for exchange of know-how in order to allow access to a larger number of scientists. This actors-partners federation is essential to reinforce the competitiveness of french teams.

The GDR will meet in plenary sessions once every 2 years. One school will be organized every two years and thematic workshops will be regularly organized.

Cover photo: Scanning electron microscopy image of a spherulite, 10 μ m in size, about to detach from a polymer (poly-lactic acid) after enzymatic attack. This image shows the difference in erosion rates between the amorphous and crystalline parts in the polymer. It illustrates the importance of the microcrystalline structure of a plastic during its degradation in the environment. © Matthieu George / Laboratoire Charles Coulomb (L2C), Université de Montpellier, CNRS / LabEx NUMEV.

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