SPMS, UMR CNRS 8580

LABORATORY STRUCTURES, PROPERTIES AND MODELING OF SOLIDS

Structures
Properties
Modeling *of*
Solids

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THEMATIC FIELDS

FERROÏCS FOR TOMORROW'S DEVICES

This research theme revolves around ferroelectric materials, which have an electrical polarization that an electric field can control, and their coupling with mechanical or magnetic commands. This theme has particularly distinguished itself in the following areas of research:

- **Neuromorphic memories and components**: The ability to control polarization using an electric field opens up new possibilities for information storage and processing devices. This work explores ferroelectric relaxor materials for less energy-intensive FE-FET memories, memristor and memcapacitor components for neural networks.
- **Nanostructures and exotic polar states**: New polar states, such as skyrmions and vortices, are being studied for low-energy memories. These topological structures emerge in dimensionally reduced ferroelectric materials (super-lattices and nanoparticles). The SPMS focuses on the characterization and simulation of these systems, with collaborations for developing thin films.
- **Electrocaloric refrigeration**: This research, in collaboration with SATIE at ENS Paris-Saclay and the Josef Stefan Institute, aims to develop lead-free materials and cascade refrigeration devices based on ceramics, polymers, and composites. Particular interest is focused on very low-temperature applications for space and quantum computing.
- **Photo-pyro-piezo-catalysis**: Ferroelectric materials can catalyse oxydation-reduction reactions using ultrasonic, thermal, and optical excitations. Research at the SPMS shows the strong piezo-catalytic and photo-piezo-catalytic potential of ferroelectric nanoparticles for degrading pollutants. Development and industrial collaboration initiatives are underway, supported by local initiatives and proof-of-concept projects.

NEW SUSTAINABLE CONVERSIONS

- **Materials for electro- and opto-mechanical actuators**: Ferroelectrics are crucial in "smart" materials for converting energy types. They enable temperature changes to generate electricity for infrared vision, energy harvesting, and solid-state cooling for quantum computers. They also convert mechanical to electrical energy for self-powered devices in various applications. We aim to find sustainable alternatives to lead-based materials and discover new energy conversion phenomena.
- **Oxides for high-power energy storage**: This research focuses on energy storage in dielectric materials thanks to their polarization hysteresis cycles, particularly in anti-ferroelectric or ferroelectric materials close to their Curie temperature. These materials, ideal for high-power applications and specific environmental conditions, provide rapid discharge and thermal stability. The main materials studied are lead-based multilayers and lead-free alternatives for greener electronics.
- **Oxides for hydrogen technologies**: Hydrogen technologies are at the core of the energy transition, playing an essential role in converting and storing chemical energy into electricity and reciprocally. We focus on the design and test of oxide materials for high-temperature Solid Oxide Cells. We use combinatorial and autonomous research methods to speed up material discovery, focusing on oxide materials for hydrogen tech, sensors, and electronics. We seek to automate material discovery and enhance our understanding of composition-property relationships.
- **Oxides for nuclear energy**: This interdisciplinary research field explores materials and phenomena crucial for nuclear energy applications. Studies focus on understanding structural phase transitions, radiation-induced effects, and electronic properties in materials used in nuclear reactors and fuel cycles. For example, research investigates

the behaviour of materials like uranium oxides and thorium oxides under irradiation, assessing changes in structure, nonstoichiometry, and microstrain.

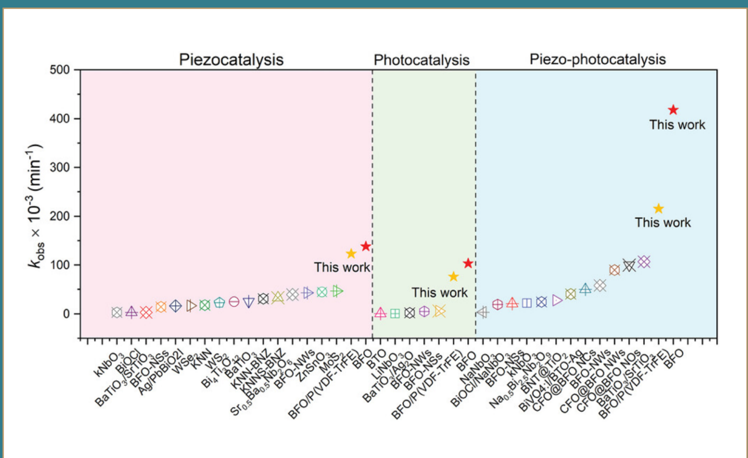
BIO-PHARMA MOLÉCULES AND MACROMOLÉCULES

- **Molecular crystals of pharmaceutical interest**: In the pharmaceutical industries, 80% of the Active Pharmaceutical Ingredients (APIs) are commercialized in solid form: either crystalline or amorphous. The formulation into a medical product of an API strongly depends on its solid form properties. There is an increasing interest in cocrystals by pharmaceutical industries. We have successfully applied the laser-induced nucleation method (NPLIN) to small organic molecules and inorganic compounds in the laboratory. We are currently testing another method using plasma excitations.
- **Physics of macromolecular complexes of biological interest**: This research aims to understand how molecular-level processes govern biological function, focusing on DNA and proteins. Spanning solid-state physics, chemistry, and bioinformatics, it uncovers key relationships between structure, dynamics, and function. Our goal is to reveal how chemical interactions, conformational changes, and atomic fluctuations orchestrate biological functions from disorder.

Application Domains

Electronic, Energy, Environment and Pharmaceutical industries, functional materials, piezoelectric transducers, energy harvesters, solid oxide fuel cells, multilayer capacitors, electrostrictive actuators, memories and artificial synapses, quantum enabling technologies, photovoltaic cells, photo- and piezo-catalysts, photo-sensors and emitters, biomedical field, hydrogen technologies, nanostructured ceramics, nuclear materials.

HIGHLIGHTS 2023



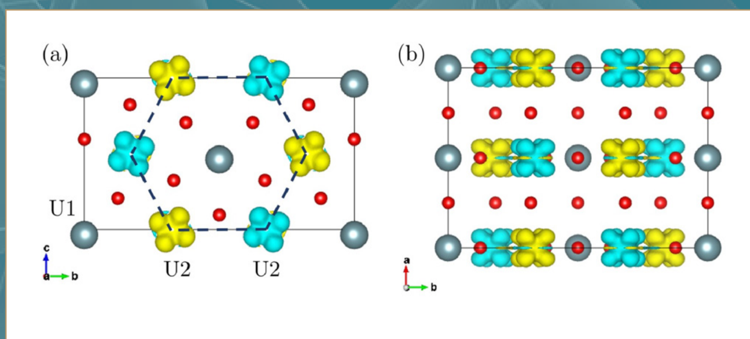
Degradation rate constant kobs for various materials. BFO (red stars) and BFO/P(VDF-TrFE) (orange stars) piezo, photo and piezo-photocatalytic activities compared with other ferro/piezoelectric materials.

$BiFeO_3$ nanoparticles for record efficiency in piezo-photo-catalysis

$BiFeO_3$ nanoparticles synthesized by an innovative method demonstrate exceptional efficiency in piezo-catalysis and piezo-photo-catalysis. As catalysts, they enable rapid degradation of organic pollutants under sunlight and mechanical vibrations, surpassing conventional methods. Integrating these nanoparticles into a polymer flm ensures efficient reuse and limits secondary pollution, opening up new avenues for diverse applications, from pollution control to hydrogen production and medical therapy. [W. Amdouni et al., Angew. Chem. Int. Ed. 62,e202215700 (2023); W. Amdouni et al., Adv. Mater. 35, 2301841 (2023)].

Charge order and spin order in U_3O_8

Yellowcake (U_3O_8), a uranium concentrate powder from leaching solutions, is a crucial intermediate in uranium ore processing for nuclear fuel production. Despite its signifcance, understanding the low-temperature magnetic order and electronic properties of U_3O_8 remained inconclusive. Through the reinterpretation of neutron scattering results and employing group representation theory, we established that its ground state displays collinear magnetic moments, both within and between layers, relieving geometric frustration. This generates a slightly distorted honeycomb lattice with Neel-type antiferromagnetic order. Precise knowledge of this magnetic ground state elucidates the system's band gap characteristics. Spin-orbit coupling (SOC) plays a critical role, signifcantly altering the electronic structure by reducing the gap by approximately 38%. The predicted electronic structure aligns well with recent optical absorption measurements, highlighting agreement between calculated and experimental properties. [Phys. Rev. Materials 7, 054410 – 2023]



Magnetization density along the direction of the a axis. Gold indicates a positive magnetization and cyan a negative one. (a) Top view of the orthorhombic unit cell. This shows the in-plane honeycomb Néel-type AFM order. (b) Side view of the unit cell, showing the interlayer AFM coupling. This strongly suggests a type of superexchange mechanism mediated by the oxygen atoms between the U2 atoms.

Industrial Partners

- COORSTEK
- EXXELIA
- FERROPERM
- HORIBA-JOBIN YVON
- IMASONIC
- IXSEA (SONAR)
- LETI
- NANOE
- PYTHEAS TECHNOLOGY
- SAINT-GOBAIN
- SCHLUMBERGER
- ST MICROELECTRONICS
- SRT Microcéramique
- THALES & THALES UNDERWATER SYSTEMS

Academic Partners

NATIONAL: CEA-Saclay, CEA-DAM, CEA-Cadarache, Faculty of Pharmacy (Paris-Saclay), ICMCB, ESRF, SOLEIL, LETI, Thiais, Vitry, ENS-Paris-Saclay, C2N-Saclay, UMPhy-Saclay, GEMAC-Versailles, GREMAN-Tours, IMMM-Le Mans, UPJV-Amiens, etc.

INTERNATIONAL: University of Tokyo Waseda, Spring8, University of Arkansas, EPFL, University of Cracaw, University of Belgrade, University of Barcelona, Georgia Tech, JSI-Slovenia, Univ. Duisburg-Essen-Germany, LIST&Univ-Luxembourg, Univ. Liège-Belgium, UCLondon-UK, ISIS-UK, NTNU-Norway, Univ. Tunis El Manar-Tunisia, Xi'an Jiatong Univ-China, East China Normal Univ.-China, SITP-Shanghai-China, UDrexel-USA, UC Berkeley-USA, UConn-USA, etc.

Key figures

• Professors, Associate Professors & Researchers	21
• Engineers & Administrative staff	11
• PhD Students	12
• PostDocs	6
• Visiting Professors	3
• Publications of the year (WoS)	44

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