

1. Objectives of the project:

Supramolecular self-assembly has been extensively studied as a way of tuning the properties of molecule-based materials. Liquid crystals (LCs), which combine order and mobility, exhibit intrinsic high sensitivity to various external stimuli, including light, temperature, mechanical shear, electric field, magnetic field, and surface interactions with foreign molecules. The incorporation of rationally designed building blocks (photo, electro, ionic) into the LC system allows for obtaining **multifunctional liquid crystals** with interesting prospects as **stimuli-responsive materials** (Figure).

The aim of this project is to develop new liquid crystal materials that can respond to various signals. This will be achieved by combining specific units with polyoxometalates

(POMs), which are intricate molecules composed of metal atoms, such as tungsten or molybdenum, surrounded by oxygen atoms. This combination will give rise to new LC-POM hybrid materials. Several methods will be studied, including covalently bonding them and incorporating them into polymers using a specialized technique. This project will also explore a multilevel functionalization of LC-POM hybrids by encapsulating POM with organic cations capable of chelating metallic systems.

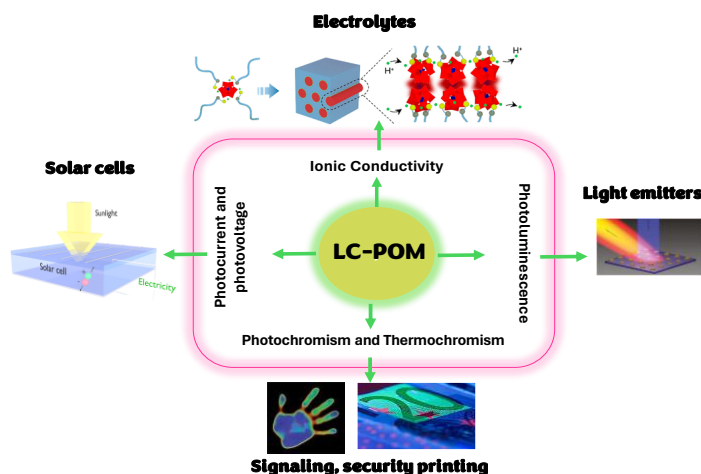


Figure. General objectives of the project

2. Research to be carried out:

The activities planned in the project can be summarized as follows:

- 1) Development of synthetic strategies with emphasis on pre-programmed and well-defined complexes using covalent and ionic functionalization, both with mesogenic units.
- 2) Design and exploration of hybrid LC-POM polymeric systems synthesized by ATRP using POM either as an initiator or as a macromolecule.
- 3) Structure characterization and analysis of the supramolecular and/or liquid crystal organization.
- 4) Evaluation of the response to stimuli to characterize their viability as functional materials in the LC phase:
 - a) Photoluminescence (light emitter concept)
 - b) Voltage and current response to sample irradiation (solar cells concept)
 - c) Induction of liquid crystal phase by light pulse and subsequent color change. Study of subsequent perturbation by heat, light, shear, redox (photochromism concept and self-healing)
 - d) In the case of compounds formed by encapsulation, these systems will be evaluated as potential electrolytes.

3. Reasons for choosing the research topic:

The integration of nanoscale **POMs into LCs** results in the development of innovative functional liquid-crystalline nanomaterials, which gained increasing prominence in recent years. The LC-POM hybrids are typically obtained by encapsulating the anionic POM with an organic ligand. However, covalent functionalization, although only a few examples are reported, offers significant advantages over ionic analogs due to its greater control of self-assembly and potential stability. To date, no liquid crystal polymer containing POM hybrids has been reported, despite it being one of the most explored strategies in the field of liquid crystals. The reported works using POM as stimuli-responsive materials have mostly been studied in solution, and these results may not be the same in the solid phase, because in most cases, response times are shorter in solution than in the solid state. For solid-phase applications, the embedding of POM in organic thin films is one of the most explored methods. However, one of the challenges in stimuli-responsive materials is the restricted mobility of building blocks within the network, which results in significant spatial limitations, imposing limits to achieve stimuli-responsiveness.

4. The most important expected effects

The main hypothesis is that by strategically modifying these systems to exhibit liquid crystal properties, will allow for response times to external stimuli similar to those obtained in solution while retaining the advantages of their easy incorporation into future devices due to their non-liquid nature. Also, due to the ionic and organized nature of the encapsulated LC-POMs, these dual systems will be evaluated as potential high-performance electrolytes that may offer a new route to design advanced ion transport systems for energy and electronic applications in solid state.