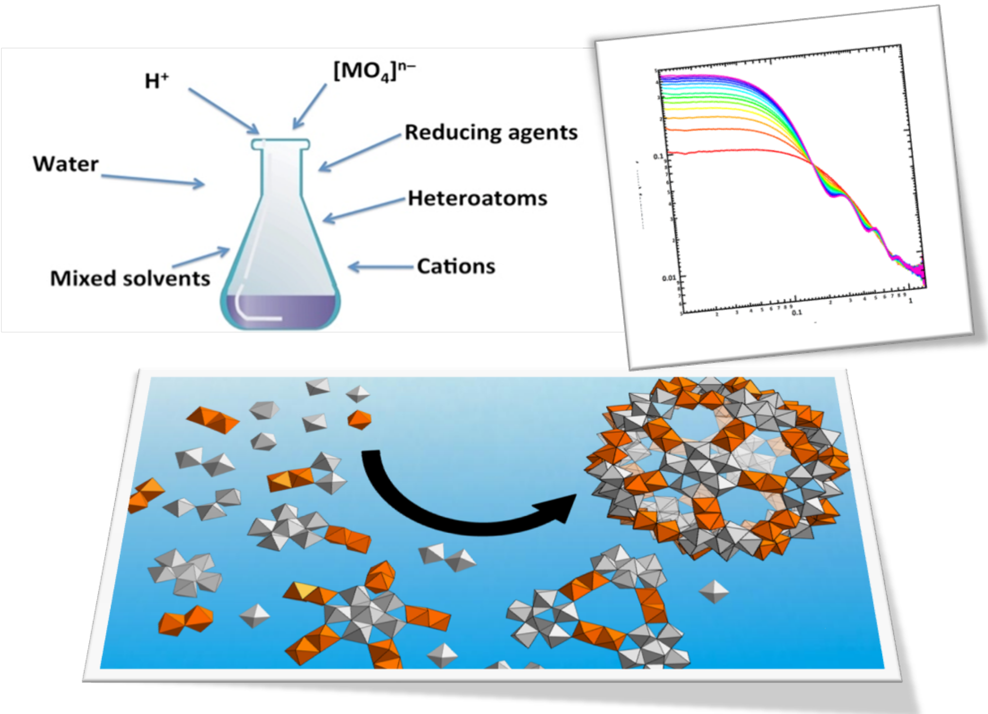
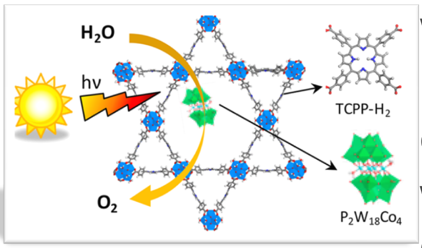
SCIENTIFIC TOPICS

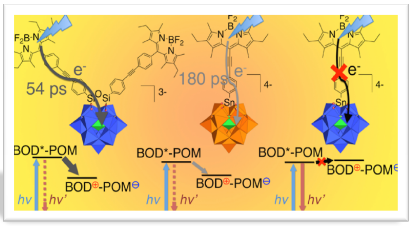
WG1 Advanced tools in synthesis, characterization and modelling

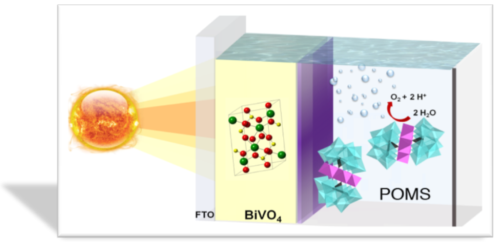


Synthesis is at the heart of the IRNPOM, therefore WG1 is transversal and will feed the three other WGs. We can rely on a strong background in synthesis that allows us to provide tailored made POMs for a variety of targeted applications. The extreme diversity of POM molecular structures and related properties will be fully exploited. The important mission of this WG is to collate reliable and validated procedures in order to pass on the accumulated knowledge and skills in POM synthesis while further expanding capabilities and understanding. The mechanism of formation and aggregation of larger POMs is under active investigation, combining various characterization techniques that had been little used in POM chemistry until now (e.g. mass spectrometry, X-ray and neutron scattering) and theoretical calculations and this will improve our ability to control the assembly of POM-based molecular structures of increased complexity (see WG4).

WG2 Catalysis, energy and environmental applications





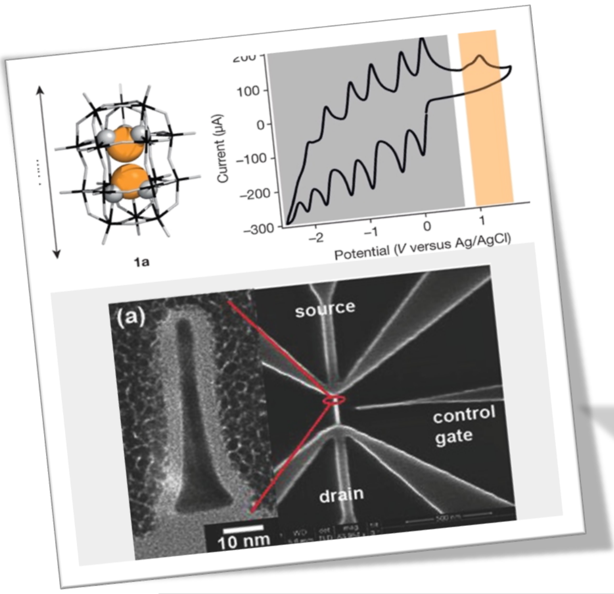


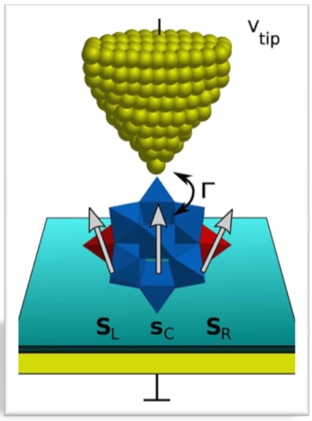
With regard to the major societal issues of chemical sustainability and energy security, we have very recently witnessed renewed activity related to green chemistry, artificial photosynthesis and energy storage. Transition-metal derivatives of POMs have been proven to catalyze water oxidation under various conditions. The reverse reaction, i.e. oxygen reduction in fuel cells is also catalyzed by POMs. While electro-assisted water reduction by POMs is well illustrated, CO2 reduction to fuels, biomass conversion, and liquefaction of natural gas remain more challenging and require greater efforts. Most often oxidation and reduction processes are studied independently from each other and electrochemical or photo-electrochemical cells that combine both aspects still require extensive design. In the field of energy storage, POMs have also been used in molecular cluster batteries and supercapacitors. Therefore, the challenges we are facing are manifold:

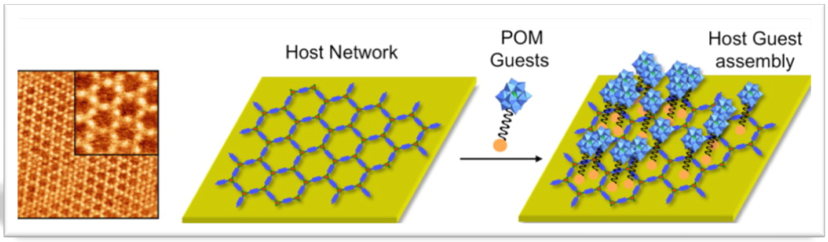
- to improve the stability and efficiency of POM-based molecular systems to compete with bulk materials.
- to devise a wider range of POM-photo-sensitizers dyads that are able to harvest solar energy
- to further the design and innovation in POM-based modified electrodes (including photo-electrodes) and their characterization and move ahead with their integration into a prototype of a complete cell.
- to rationalize the advantages of POMs to move forward in battery and supercapacitor technology, for example, towards redox flow batteries.

WG3 Information technologies

Data storage and information processing at the molecular scale is a response to the continuous drive towards reduction in electronic /magnetic components size. Electro-active molecules that can be switched from one redox state to another have been proposed for the development of molecular memory devices and POMs that display discrete, reversible, mono- or multi-electronic states are promising candidates for multi-level digital data storage. The magnetic properties of transition metal substituted POMs make also these molecules of interest in Quantum Technologies as robust spin qubits and quantum gates. The interest of these electroactive molecules in molecular electronics has recently expanded to their use in spin electronics (spintronics), and molecular spin valves incorporating POMs have been envisoned. However, the challenges are now:

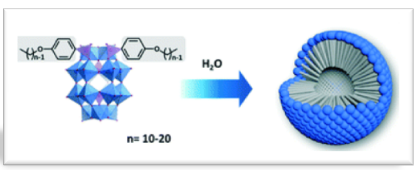


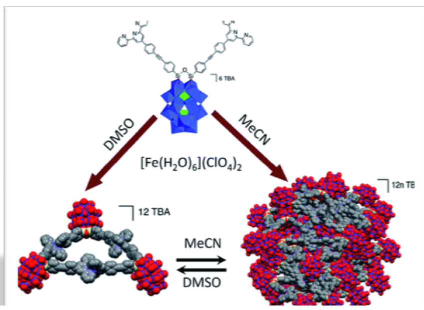




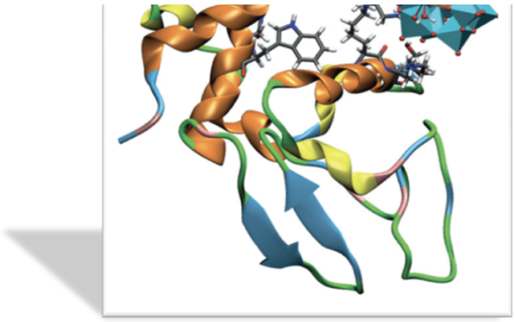
- to devise molecular junctions at various scales from the processing and characterization of large assemblies of regularly dispersed POMs on solid surfaces to the manipulation of single POMs.
- to improve the performance of the devices by a better engineering of the molecules /electrode interface
- to enlarge examples of POMs integrated in solid-state components

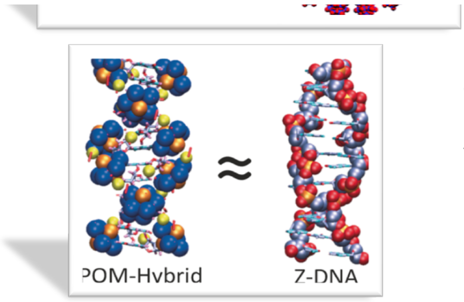
WG4 Mimicking nature's complexity





POMs have found many applications in fields ranging from biology to functional materials, where they have been





used either in solution, deposited onto various substrates or as bulk materials. In most cases little attention has been paid to the intermolecular POM-to-POM interactions or to the interactions of POMs with their substrates or more generally their surroundings. However, recent studies of the self-assembly of POM macroions into blackberry structures through counter-cation mediated attraction and the formation of micelles, hollow vesicles or liquid-crystal phases by self-assembly of amphiphilic POM hybrids driven by solvophobic interactions open new perspectives to devise innovative ‘soft’ materials with POMs embedded as functional components. Supramolecular chemistry provides powerful tools to build large assemblies with hierarchical organization, as encounters in nature in order to optimize the sought functions. This should inspire us to move forward and design complex self-assemblies based on POM building blocks that can be further triggered by external stimuli (medium polarity, light, pressure and reducing agent, among others). Emerging properties arising from the dynamic structural complexity are expected. Confinement or compartmentalization inside such materials will also improve catalytic processes, charge separation or transport, or provide cargos for the delivery of biologically active molecules.