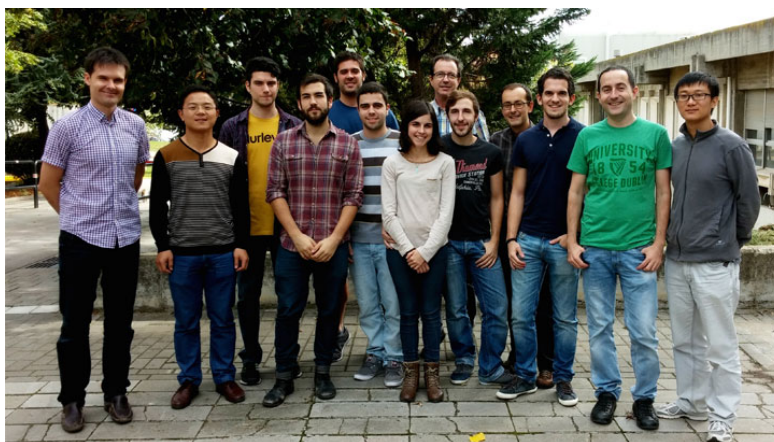


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Selective Oxidation Catalysis Research Group (SelOxCat)



The energy demand of modern societies is increasingly high, while the reserves of non-renewable fuel sources, the most common, are diminishing. In this situation, the search for renewable energy sources acquires considerable importance. The SelOxCat research group uses a range of techniques to study, understand and develop the reactions leading to the production of renewable fuels from water and sunlight.

The [SelOxCat research group](#) focuses on the design and preparation of molecular or colloidal systems based on transition metal and hybrid materials to be applied as oxidation-reduction catalysts. Particularly, the group is interested in the study, comprehension and development of key reactions for the production of renewable fuels from water and sunlight, such as the oxidation of water to dioxygen and the reduction of protons to hydrogen gas or the reduction of carbon dioxide to methanol or methane gas. It uses a wide range of techniques, including spectroscopy, electrochemistry, electronic microscopy and X-ray crystallography, in order to understand these processes at the molecular or atomic level.

The group was founded in 2011 within the Department of Chemistry of the UAB. It is currently led by the lecturers from the area of Inorganic Chemistry Xavier Sala, Jordi García-Antón, Roger Bofill and Lluís Escriche and includes five PhD students (Rosa Gonzalez, Jonathan De Tovar, Mark Gil, Jordi Creus, Bing Jiang), a masters student (Lluís Solà) and four undergraduate

students.

Research Lines

The research conducted by SelOxCat is divided into three main lines:

Selective and sustainable oxidative transformations. Among the oxygenated products, epoxides (organic molecules formed by a ring of three atoms containing one oxygen atom) are of central importance in organic synthesis since they provide access to highly diverse molecules by means of subsequent transformations. In addition, their chiral derivatives (molecules that have the property of not being superimposable with their mirror image) constitute versatile intermediates for the synthesis of numerous natural products and biologically active substances. However, the most common methods of preparation are still based on the use of rather expensive oxygen-atom transfer oxidants or high loadings of toxic metals. Therefore, to develop selective/enantioselective (i.e., to distinguish between a molecule chiral and its enantiomer, which is another molecule given that it is the mirror image which is not superimposable on the first) and sustainable methodologies for preparing these epoxides is the main goal of this research project.

New energy conversion schemes. Artificial photosynthesis. The dissociation of water by sunlight is an attractive alternative to photosynthesis, since it is a very clean and simple reaction from a chemical point of view. This process, called artificial photosynthesis, is based on the use of non-protein synthetic catalysts for the oxidation of water to molecular oxygen and reduction of water protons in hydrogen gas (high performance fuel) or reduction of atmospheric CO₂ in energetic or synthetically useful (methane, methanol, formaldehyde, etc.) products. The overall objective of the group is to generate clean energy from water and sunlight by means of catalytic reactions harmoniously combined in a photoelectrochemical cell.

Use of nanoparticles in catalysis. Surface chemistry. The processes described above can also be carried out by means of nanosized materials (colloids, usually transition metals) stabilized by molecules attached to the surface (called ligands). The goal of this research line is based on the molecular characterization of nanoparticle-ligand interactions at the molecular level using spectroscopic techniques (NMR essentially) during the oxidative changes described above.

Selected publications from the past three years

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