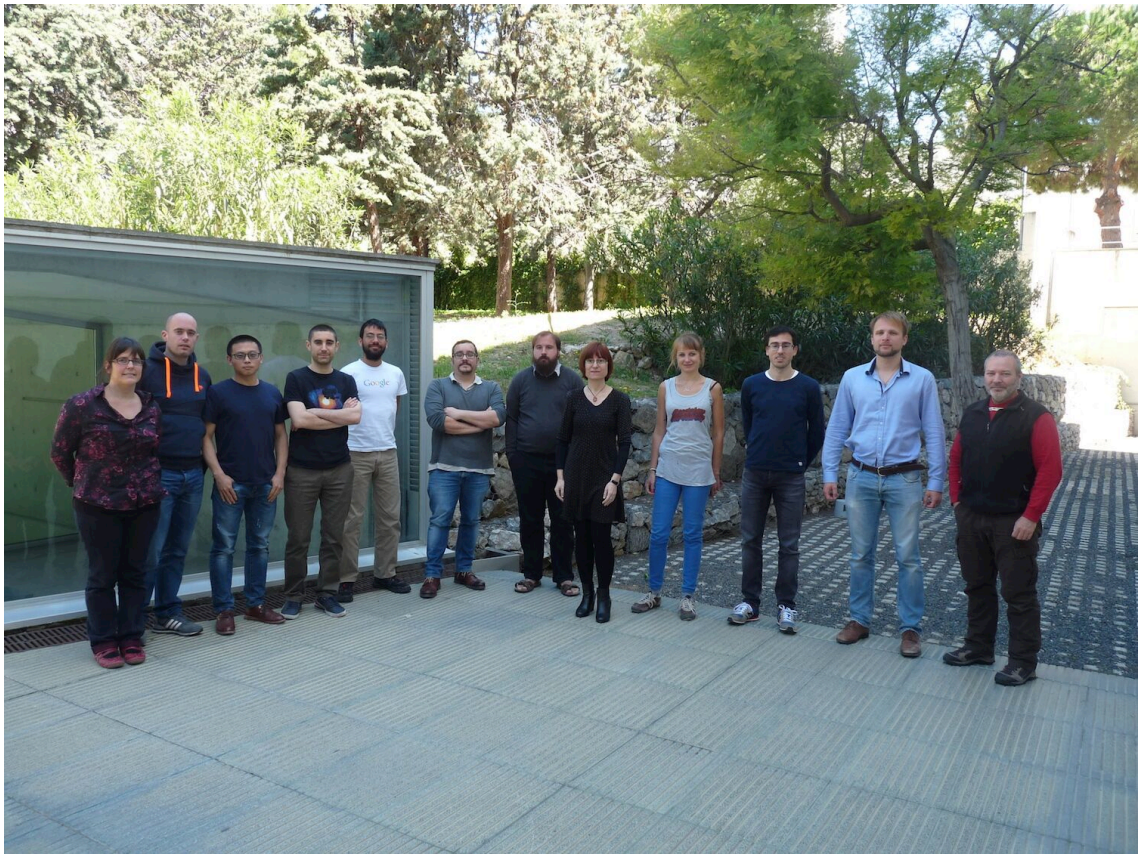
López Research Group



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Abstract

The aim of the group is to employ atomistic simulations to understand the mechanisms that govern chemical processes in heterogeneous catalysis and other materials that might be appealing due to their ability to extract, store or provide energy. Both the analysis of reaction networks, activity and selectivity issues and the final tests on the stability of the potential materials are fundamental to establish a solid background to determine the potentialities of catalyst candidates for a given chemical transformation. As for the new energy materials their performance and stability are two of the main goals in our research.
Our collaboration with several experimental groups is of fundamental importance to define and compare models that can later be applied to suggest experiments and new materials to be explored. To this end, the use of massive computational resources, as those provided by the RES-BSC is required. We are thankful to them for these resources that help in placing us as players at the European level.

Following our previous research we have been working on different areas of theoretical simulations on catalytic properties of materials.

We have investigated the dynamic properties of Metal-Organic Frameworks. The main contributions are they lability against solvents that allows the metal exchange in the transmetallation process and the fact that they cannot be considered as well-defined materials in terms of coordination as the materials always store some solvent. These two publications have been presented in Chemistry of Materials and ACS Central Science and the later was presented in the ACS in San Diego.

A second type of studies have been devoted to the study of water metal interfaces for the Ru(0001) this is in line with our studies on the reactivity of biomass-derived molecules for their use as chemicals platforms. In this last point we have considered a set of transformations mainly of methanol on both metal and oxides and we have achieved a large degree of understanding on the problem. While metals can decompose the material leading to CO and hydrogen on oxides the reaction can be controlled and stopped at formaldehyde. These results have been published in the best Catalysis journals including ACS Catal., J. Catal. and ChemSusChem. In addition, we have observed that it is possible to define a new set of not-energy based descriptors that can in a continuous manner be employed to unravel complex chemistries in complex materials.

We have also kept our collaborations with other groups in particular with Prof. Javier Pérez-Ramírez in the area of hydrogenations. Two important investigations in the area of decorated nanoparticles and single site catalysis have emerged. The results have been published in ACS catalysis and Angew. Chem. Int. Ed.
How single atom modifies the environment in a molecule has also been investigated for dyes. In collaboration with the group of Prof. Emilio Palomares we investigated the modifications induced by a single atom in a long-chain complex dye. Changes in the electronic structure and the relative dipoles when interacting with the titania surface are at the basis of such interesting behavior. The results have been published in Energ. Env. Sci.

Through a collaboration with REPSOL we investigated a different type of isolated centers that are very attractive for the synthesis of polyols in double metal cyanides. The structures of these materials are complex and very dynamic and the reaction mechanism was investigated for the first time employing state-of-the-art methodologies. Our seminal work will open new research areas in complex amorphous materials for industrially relevant reactions.

The shape of active catalytic materials was reviewed by computational techniques showing the potentialities of atomic Wulff constructions. An important size-ensemble effect was observed and we believe that any complex simulation that takes into account the counting of active sites will require this type of approach in the future.

Finally, we have been very active in the development of standards for the storage of computational data, the BigData4Cat project. We have now running a platform that serves to store in an ordered manner the data produced in our lab and we are now searching for a potential way to intensively mine this datasets.

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