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**Research and short biography**

M. Rosa Axet research activities are focused in the organometallic and nanomaterials chemistry areas, for applications in catalysis. She is interested in the study of the structure-properties relationships in several nanomaterials including bimetallic, supported or shape-controlled nano-objects, with special attention to the effects of the stabilizing ligands of the nanoparticles on their properties. Her PhD was essentially focused on chiral homogeneous catalysis for hydroformylation with a first experience with nanomaterials (Rovira i Virgili University, Tarragona, Spain, supervised by Carmen Claver and Sergio Castillon), which was further developed in her postdoctoral position with Bruno Chaudret (LCC-Toulouse, France). She had the opportunity to work as well with Hani Amouri (IPCM, Paris, France), and Barbara Milani (Trieste, Italy), both as a postdoc. She joined the CNRS as an associate researcher in 2010. Since then, she has developed a research on the field of nanocatalysis. She is co-author of 40 articles, 5 book chapters, and 1 patent. She was awarded in 2019 with EMERGENCE@International INC-CNRS (Japan, 18<sup>th</sup>-30<sup>th</sup> November 2019).

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## Adsorbate effects on metal nanoparticles, from synthesis of bimetallic systems and 3d assemblies of nanoparticles to the impact on catalysis

Intrinsic properties of metals determine adsorption energies on their surfaces, which is extremely important to understand the catalytic properties of metal based catalysts. Theoretical methods have allowed to rationalize these properties by finding correlations as scaling relationships, volcano plots and cliff shapes.<sup>[1]</sup> In order to circumvent these dependencies it is essential to break the scaling relationships by creating complexity in the catalytic materials.<sup>[1]</sup> Several strategies have been emerged in the last years, including alloyed systems, single-atom catalysts, modification of the metallic surface with adsorbates, among others, which have permitted to access new reactivities, and to certain extent to bridge the gap between the classically labelled heterogeneous and homogeneous catalysis fields.

In our research, intertwining theoretical and experimental work, we have focused on the modification of metallic surfaces by the addition of a second metal, a coordinating ligand, or a combination of both, to understand the effect of these adsorbates in the outcome of the catalytic reactions; additionally, we have explored the reactivity of single-atom materials as catalysts. In this sense we have developed a family of hybrid materials, allowing obtaining from ultra-small Ru NP to ordered materials in a precise manner.<sup>[2]</sup> Also, the control of the electronic properties of the ligands present on the surface allows to understand and modulate the activity and selectivity of ruthenium NP used as catalysts in several hydrogenation reactions.<sup>[3, 4]</sup> Finally, ruthenium nanoparticles can be finely tuned by adding a second non precious metal. These bimetallic nanoparticles have been successfully used as catalysts in the selective 5-hydroxymethylfurfural hydrogenation, which is a promising intermediate for the synthesis of a wide variety of chemicals and alternative fuels based on bio-refinery.<sup>[5]</sup>

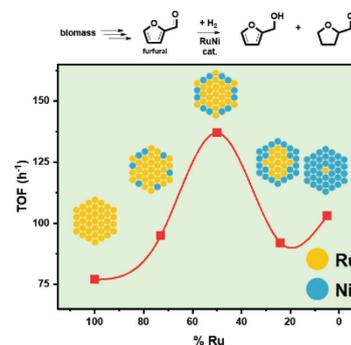


Figure 1. Synergistic effect of Ru-Ni bimetallic nanocatalyst

## References

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