

### **1. Interested institution:**

The Spanish National Research Council (CSIC)

C/ Serrano 117, 28006, Madrid (Spain)

[www.csic.es](http://www.csic.es)

### **2. Brief Description of the Institution**

The Spanish National Research Council (CSIC) is the largest public institution dedicated to research in Spain and the third largest in Europe. Belonging to the Spanish Ministry of Economy and Competitiveness through the Secretary of State for Research, Development and Innovation, its main objective is to develop and promote research that will help bring about scientific and technological progress, and it is prepared to collaborate with Spanish and foreign entities in order to achieve this aim. It has a staff of more than 13,000 employees, among these about 3,300 are permanent researchers and about 4,300 are pre- and post-doctoral researchers. The CSIC has 70 fully own institutes or centres distributed throughout Spain. In addition, it has 53 Joint Research Units with universities or other research institutions. There is also a delegation in Brussels and Rome.

CSIC has considerable experience in both participating and managing R&D projects and training of research personnel. Under the 7th Framework Programme CSIC has signed approximately 700 actions (including 97 coordinated by CSIC and 47 ERC projects). Funding wise, CSIC is listed the 1st organisation in Spain and the 5th in Europe in the 7th Framework Programme, with a total FP7 contribution of over 260 million euros. During the first calls of H2020, CSIC has had an intense participation in all programmes. It has been remarkable the participation in certain calls, such as ERC and Marie Curie, as well as in ICT, NMBP and Societal Challenges. In March 2015 CSIC has obtained 90 projects with a total financial contribution of 40 million euros.

### **3. Please tick the areas of research (as established in Marie Skłodowska Curie Actions)**

- |                                                                    |                                                                   |
|--------------------------------------------------------------------|-------------------------------------------------------------------|
| <input checked="" type="checkbox"/> Chemistry (CHE)                | <input type="checkbox"/> Environmental Sciences and Geology (ENV) |
| <input type="checkbox"/> Social Sciences and Humanities (SOC)      | <input type="checkbox"/> Life Sciences (LIF)                      |
| <input type="checkbox"/> Economic Sciences (ECO)                   | <input type="checkbox"/> Mathematics (MAT)                        |
| <input type="checkbox"/> Information Science and Engineering (ENG) | <input type="checkbox"/> Physics (PHY)                            |

#### **4. Research / Project Description**

**Title:** Polyhedral Boron-based metal clusters in the activation and modification of small molecules

This proposal is concerned with the development and study of polyhedral boron-based clusters of utility in the activation of small molecules, focused on their modification through catalytic cycles.

In recent years, we have developed convenient synthetic routes to 12-, 11- and 10-vertex polyhedral boron-based metal clusters that have allowed the systematic study of their reaction chemistry. Salient aspects of our research are: (i) the first examples of dihydrogen activation on polyhedral clusters in a reversible fashion (Álvarez *et al.* *J. Am. Chem. Soc.* **2008**, 130, 2148; Calvo *et al.* *Chem. Commun.* **2013**, 49, 9863), (ii) oxidative addition of *sp* C–H bonds (Álvarez *et al.* *Chem. Eur. J.*, **2009**, 15, 5428), (iii) catalysis of hydrogenation and isomerization of olefins (Álvarez *et al.* *J. Am. Chem. Soc.*, **2008**, 130, 11455), (iv) hydrosilylation of terminal alkynes with high  $\alpha$ -selectivity (Susana Luaces Thesis, to be presented), (v) reversible photorelease of O<sub>2</sub>, CO and SO<sub>2</sub> from the 12-vertex platinaborane (Bould *et al.* *Inorg. Chem.* **2011**, 50, 7511), (vi) construction of SAMs composed of metallaboranes and bimetallaboranes (Bould *et al.* *Inorg. Chem.* **2012**, 51, 1685), (vii) preparation of polyhedral cations with high redox / structural flexibility (Calvo *et al.* *Organometallics* **2012**, 31, 2526; *Chem. Eur. J.* **2013**, 19, 3905; *Dalton Trans.* **2014**, 43, 5112). The reactivity found in the studies quoted above is the result of the mutually synergistic interaction of metal on heteroborane moieties and heteroborane ligands on metal centers, leading to classical *closo-nido-aracno* structural transformations. This chemical behaviour is somehow reminiscent of the metal-ligand cooperation found in, for example, the ubiquitous pincer ligands in that the heteroborane moiety, viewed as a ligand, takes part in the reaction. This synergy is, however, more intimate in the polyhedral clusters due to the quasi-aromatic delocalized nature of the skeletal bonding. As structure determines the properties, these polyhedral clusters have the unique capability of responding in a concerted manner to perturbations that can start at any of the vertices: the metal centre, the B–H units or the heteroatom (for example, S or C).

We are able now to form active polyhedral clusters by the chemical modification of the ligands at the metal centre and at the boron vertices, and by simple protonation of the cages; and since the highly delocalized three-dimensional cluster bonding contributes decisively to observed reactivity, we propose photochemical and electrochemical methods for the formation of excited metallaheteroboranes (formation of “active clusters”) and to use them in the activation of small molecules such as H<sub>2</sub>, O<sub>2</sub>, NH<sub>3</sub> and CO<sub>2</sub>.

##### **Group**

The applicant will be incorporated into the research group Homogeneous Catalysis by Organometallic Compounds of the Instituto de Síntesis Química y Catálisis Homogénea (ISQCH). The research group is lead by Prof. Luis A. Oro, (Highly Cited Researcher, <http://sorores.unizar.es/personales/LAO/oro.html>) and is formed by 10 permanent scientists of the University of Zaragoza and of the CSIC, as well as a number of pre-doctoral and post-doc researchers of different nationalities. The group possesses extensive experience in Organometallic Chemistry and in Homogeneous Catalysis having published more than one hundred research papers in international journals of recognized international prestige in the last five years. The

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general aim of the research activity of the group is the development of new transition metal organometallic compounds and its applications as homogeneous catalysts including the immobilization on different solid supports. The group is currently financed by competitive research projects from public institutions as well as contracts with chemical companies. The group is responsible for academic and research training at all the University levels.

### ***5. Who can apply?***

At the deadline for the submission of proposals (10/09/2015), researchers (\*):

- shall be in possession of a doctoral degree or have at least four years of full-time equivalent research experience.
- must not have resided or carried out their main activities in the country of Spain for more than 12 months in the 3 years immediately prior to the abovementioned deadline.

### ***6. Contact person***

Dr. Ramón Macías  
e-mail: rmacias@unizar.es

### ***7. Applications: documents to be submitted and deadlines***

- CV
- Letter of motivation
- Two recommendation letters
- Dead line of application: June, 15<sup>th</sup> 2015.

Please note that:

- Deadline of the next call for proposals for Marie Skłodowska – Curie Individual Fellowships is **September, 10<sup>th</sup> 2015**.
- Oficina Europea is only responsible for the display of the expressions of interests received by the institutions; further contact and information requests will take place directly between the host institutions and the interested researchers.

(\*) Further details on the Call and additional eligibility criteria can be found at the [Participants' Portal](#)