

"EXPRESSION OF INTEREST" FOR HOSTING MARIE S. CURIE FELLOWS IN SPANISH INSTITUTIONS (CALL MSCA IF 2015)

1. Interested institution:

The Spanish National Research Council (CSIC) - C/ Serrano 117, 28006, Madrid (Spain)
www.csic.es

Instituto de Síntesis Química y Catálisis Homogénea (ISQCH)
Universidad de Zaragoza-CSIC
C/ Pedro Cerbuna 12 - Zaragoza

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)

☒ **Chemistry (CHE)**

☐ Social Sciences and Humanities (SOC)

☐ Economic Sciences (ECO)

☐ Information Science and Engineering (ENG)

☐ Environmental Sciences and Geology (ENV)

☐ Life Sciences (LIF)

☐ Mathematics (MAT)

☐ Physics (PHY)

4. Research / Project Description

LED lighting technology will develop hugely within the next few years due to the incandescent phase-out. Nowadays, two main strategies are available in Solid-State Lighting (SSL) to generate white luminescence (WOLEDs):

- 1) The PC-LEDs (phosphor-converted LED). In these devices, short-wavelength emission from the LED dye is partially downconverted by the phosphors. White light results from the combination of the phosphors re-emission and LED non-absorbed light.
- 2) The RGB LED, that consists out of three emitters (primary at around 455 nm, 530 nm and 610 nm) closely together to form a compact semiconductor light source with a tunable chromaticity point.

Phosphors used in mainstream LED technology are typically inorganic, comprising most of them a crystalline oxide, nitride, oxynitride or silicate host lattice doped with a small dose of an activator ion, in most cases rare earths. Ce^{3+} and Eu^{3+} are the more broadly used in SSL. China and Russia hold the 75% of world reserves of rare earths and their export and production restrictions, with direct impact on phosphor availability and pricing, are damaging industries all over the world. In the light of this, it is clear the necessity of new phosphorescent materials capable of replacing in the next future the rare-earth based phosphors.

In the area of opto-electronic materials, conjugated organic polymers, and their molecular precursors, have shown considerable potential and devices based on these materials are now in the marketplace. However, in a purely organic light emitting device (OLEDs), emission from the triplet states is forbidden, so the efficiency is capped at 25%. This represents a huge wastage of energy, which simply goes into heating up the device. The introduction of a heavy metal atom into the conjugated organic molecule would facilitate the phenomenon of “spin orbit coupling” (SOC) which has the effect of relaxing the electronic selection rules. In this way the excited triplet states can become accessible by an “intersystem crossing” (ISC) process and then exhibit phosphorescence, reaching quantum efficiencies of up to 100%. In this field there is clearly the need for new complexes that emit efficiently at room temperature with rather short phosphorescent radiative lifetimes to avoid the loss of energy by non-radiative processes.

Within this field, square planar platinum (II) complexes containing aromatic molecules with delocalized π electron density such as diimines, terpyridines or the cyclometallated derivatives are suitable systems for these purposes because of the nature of their emissive states. The use of C,N cyclometallated imines such as 7,8-benzoquinoline (bzq) or 2-phenylpyridine (ppy) allows to achieve very efficient phosphorescent systems. The electronic features of the C- σ bond (σ donor) and the aromatic fragment (π acceptor) cause the raising of the energy of the metal centred (MC) (d-d) excited states, preventing non-radiative decay processes from occurring. These complexes normally emit from metal-to-ligand charge transfer (MLCT) and/or intra ligand (IL) excited states (Figure 1a). Emission energies (or lifetimes) can be tuned by the electron-donating or –withdrawing character of the aromatic substituents as well as by the ancillary ligands (L, L'). Such behaviour is, of course, not unique to platinum (II). Indeed, complexes of its neighbour in the periodic table, iridium (III), a d^6 metal ion, have been far more widely explored as phosphorescent dopants in OLED emitters. However, d^8 Pt(II) complexes are attractive for another reason. Their square-planar structures allow them to interact facially with one another. They may aggregate through attractive Pt–Pt or ligand–ligand intermolecular interactions or a combination of these, thereby facilitating formation of different species of higher nuclearity, called excimers and aggregates. As a consequence, a change in the nature of the emissive state is produced, now

emitting from metal-metal to ligand charge transfer (MMLCT) or excimeric ligand to ligand ($\pi\pi^*$) charge transfer (Figure 1b). Therefore, the emissions of these compounds can vary from blue-greenish (monomer; Figure 1a) to orange-reddish (aggregates or excimers; Figure 1b). All these features make them suitable phosphorescent dopants to prepare PhOLEDs and WOLEDs.

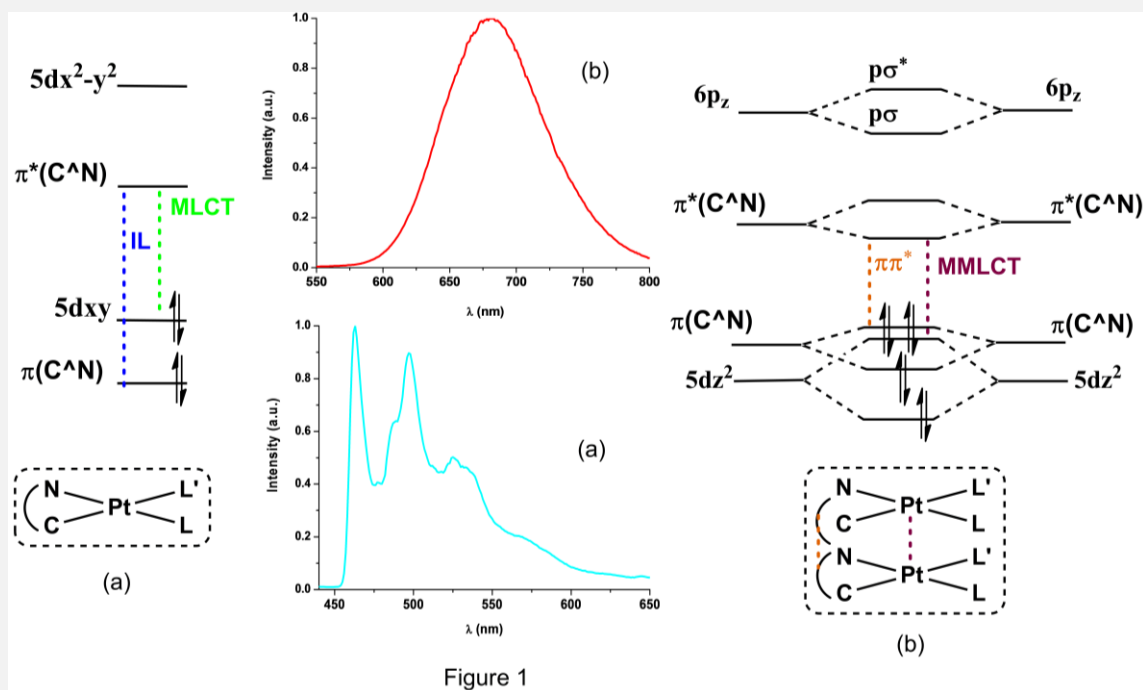


Figure 1

WOLEDs (white OLEDs) need three phosphorescent emitters (red, yellow, blue) to mimic the sun light. An example of tri-layer WOLED consists of these three phosphorescent dopants:

- Blue Iridium (III) bis(4,6-di-fluorophenyl)-pyridinato- N,C^2 picolinate [F Ir pic]
- Yellow Bis(2-phenyl benzothiazolato N,C^2) iridium (acetylacetonate) [Bt₂ Ir (acac)]
- Red Bis(2-(2'-benzo[4,5-a]thienyl)pyridinato- NC^3)iridium(acetylacetonate)[Btp₂Ir acac]

Nonetheless, discovery of technological materials that provide both operational stability and high external efficiency for the devices still remains one of the **big challenges**, particularly for emissions ranging from **blue** to **green-yellowish**. According to them, there is a break in the region of 550 nm when it comes to highly efficient PhOLEDs (Figure 2).

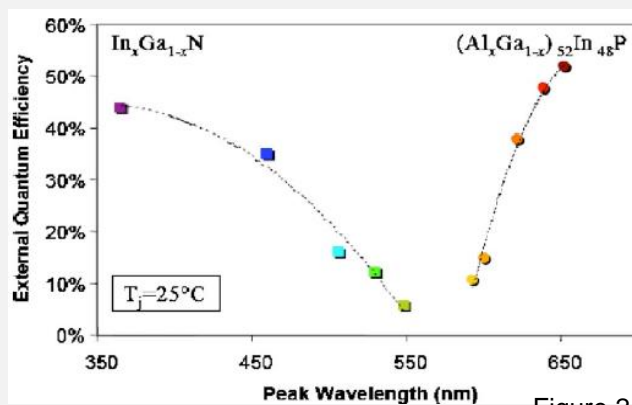


Figure 2

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Considering all these premises, the *aim* of our project could be briefly described as the **design, synthesis and characterisation of tuneable luminescent platinum, iridium and osmium compounds to be used as phosphorescent dopants in PhOLEDs and WOLEDs**. In general, complexes should display specific features for this purpose, such as a specific λ max of the emission (blue (470 nm), or green-yellowish (550 nm) or white (400 to 750 nm)), high phosphorescent quantum yields ($\Phi_p \approx 1$) and relatively short triplet lifetimes.

In addition, these complexes could undergo changes in their color and/or emission in the presence of some analytes. Because of that we will **explore their potencial use as chemosensors for optical detection of harmful species** present in the environment (heavy metal cations, anions or volatile organic compounds, VOCs).

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. Babil Menjón Ruiz
e-mail: menjon@unizar.es

7. Applications: documents to be submitted and deadlines

CV and letter of motivation

Please note that:

Deadline of the next call for proposals for Marie Skłodowska – Curie Individual Fellowships is **September, 10th 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](#)