

## Part A. Personal Information

|      |            |
|------|------------|
| DATE | 13/06/2018 |
|------|------------|

|                                      |  |                                     |
|--------------------------------------|--|-------------------------------------|
| Surname(s)                           | de Jesús Alcañiz                           |                                     |
| Forename                             | Ernesto                                    |                                     |
| Social Security, Passport, ID number | 40864541G                                  |                                     |
| Sex                                  | Male                                       |                                     |
| Age                                  | 58   |                                     |
| Researcher codes                     | WoS Researcher ID (*)                      | <a href="#">K-6107-2014</a>         |
|                                      | SCOPUS Author ID (*)                       |                                     |
|                                      | Open Researcher and Contributor ID (ORCID) | <a href="#">0000-0001-8101-1358</a> |

(\*) At least one of these is mandatory

### A.1. Current position

|                                    |  |  |
|------------------------------------|--|--|
| Post/ Professional Category        | Full Professor of Inorganic Chemistry  |  |
| UNESCO Code                        | 230321, 230326, 221001   |  |
| Key Words                          | Organometallic Chemistry, Coordination Chemistry, Homogeneous Catalysis, Transition Metals |  |
| Name of the University/Institution | Department/Centre  | Química Orgánica y Química Inorgánica  |
|                                    | Full Address   | Edificio de Farmacia, Campus Universitario, 28871 Alcalá de Henares (Madrid) |
|                                    | Email Address  | <a href="mailto:ernesto.dejesus@uah.es">ernesto.dejesus@uah.es</a>           |
|                                    | Phone Number   | 918854603  |
|                                    | Start date   | 18/12/2009   |

### A.2. Education (title, institution, date)

| Year | University        | Degree                   | Title                           |
|------|-------------------|--------------------------|---------------------------------|
| 1981 | Univ. de Zaragoza | First degree             | Licenciado en Ciencias Químicas |
|      |                   | Masters (if appropriate) |                                 |
| 1987 | Univ. de Alcalá   | PhD                      | Doctor en Ciencias Químicas     |

### A.3. Indicators of Quality in Scientific Production (See the instructions)

**Total number of citations (excluding self-citations):** 1.784

**Average number of citations (2013-2017):** 124

**Total number of publications in the first quartile (Q1):** 50

**Total number of publications in the first decile (D1):** 13

**Average Citations per Article:** 22.58

**h-Index:** 25 (ISI Web)

**Thesis supervised:** 10

## Part B. Free Summary of CV (Max. of 3.500 characters, including spaces)

My research training started during my degree studies in the group of Antonio Laguna and Rafael Usón of the University of Zaragoza with the preparation of organometallic complexes of Ti and Au. In 1983, I moved to the Universidad de Alcalá to perform doctoral studies about the synthesis and structural characterization of molybdenum and tungsten alkyl complexes under supervision of Amelio Vázquez and Pascual Royo. Between 1987 and 1989, I did postdoctoral studies in the group of Pierre Braunstein (University of Strasbourg-CNRS), where I worked on the synthesis and reactivity of heterometallic clusters. In this period, I developed new methodologies for the rational synthesis of heterodimetallic complexes with phosphide bridges based on the concept of isolobal analogies developed by R. Hoffmann. In 1990, I made a new stay of three months in the same university to perform studies on computational quantum chemistry in the group directed by Alain Dedieu. After my definitive reincorporation to the University of Alcalá in 1992 as an Assistant Professor, I developed studies on the preparation and reactivity of molybdenum and tungsten bimetallic complexes in the group of Pascual Royo.

In 1997, I started an independent scientific career initially centered in the chemistry of metal-functionalized dendrimers, being one of the first groups to study the chemistry of dendrimers in Spain. The group has been funded since 1998 by the National R & D Plans (7 projects, see C2.1-3 for the last 5 years) and by the Regional R & D Plan of the Community of Madrid. Our field of interest was initially focused on the applications of transition metal dendrimers in catalysis. In the last 10 years, our research has addressed different issues related to the recovery of organometallic catalysts (catalysts supported on dendrimers or other types of nanosystems, publication C1.5 or patents C4.1-2) and the organometallic chemistry and catalysis in aqueous phase. In this field, we have made some contributions to the development of C-C coupling processes, including mechanistic studies that have allowed us to understand the influence of aqueous solvent in some of these reactions (C1.10). We have been one of the first groups to be interested in the synthesis, reactivity and applications of water-soluble complexes with N-heterocyclic carbene ligands, having focused our work on Pd and Pt (publications C1.3,7,9). Thus, we have reported one of the most efficient Pd catalysts for cross-coupling reactions in aqueous phase (C1.6). In addition, we demonstrated for the first time that it is possible to stabilize metallic nanoparticles in aqueous solution by protecting their surface with hydrophilic NHC ligands (C1.1,2,4,8).

Our current research interests include the development of metal nanoparticles functionalized with chiral NHC ligands, the development of open shell 4d and 5d transition metal complexes, and the development of organometallic reactions in aqueous-phase.

## Part C. Relevant accomplishments

### C.1. Publications

1. J. M. Asensio, S. Tricard, Y. Coppel, R. Andrés, B. Chaudret, E. de Jesús, Knight Shift in  $^{13}\text{C}$  NMR Resonances Confirms the Coordination of N-Heterocyclic Carbene Ligands to Water-Soluble Palladium Nanoparticles, [\*Angew. Chem. Int. Ed.\* \*\*56\*\*, 865-860 \(2017\)](#). Times cited: 10
2. J. M. Asensio, S. Tricard, Y. Coppel, R. Andrés, B. Chaudret, E. de Jesús, Synthesis of Water-Soluble Palladium Nanoparticles Stabilized by Sulfonated N-Heterocyclic Carbenes, [\*Chem. Eur. J.\* \*\*23\*\*, 13435–13444 \(2017\)](#). Hot Chem Eur J Paper. [Highlighted in ChemViews Magazine](#). Times cited: 1
3. J. M. Asensio, R. Andrés, P. Gómez-Sal, E. de Jesús, Synthesis, Characterization, and Reactivity of Water-Soluble N-Heterocyclic Carbene Allyl Palladium(II) Complexes [\*Organometallics\* \*\*36\*\*, 4191–4201 \(2017\)](#). 4. L. M. Martínez-Prieto, E. A. Baquero, J. C. Flores, E. de Jesús, G. Pieters, P. W. N. M. van Leeuwen, G. Lippens, B. Chaudret, Monitoring Nanoparticle Reactivity in Solution: Interaction of L-lysine and Ru Nanoparticles Probed by Chemical Shift Perturbation parallels regioselective H/D exchange, [\*Chem. Comm.\* \*\*53\*\*, 5850-5853 \(2017\)](#). Times cited: 5.

5. A. Ortiz, A. Sánchez-Méndez, E. de Jesús, J. C. Flores, P. Gómez-Sal, F. Mendicuti. Poly(benzyl ether) Dendrimers Functionalized at the Core with Palladium Bis(N-Heterocyclic Carbene) Complexes as Catalysts for the Heck Coupling Reaction. [\*Inorg. Chem.\* \*\*55\*\*, 1304–1314 \(2016\)](#). Times cited: 4.
6. R. Garrido, Roberto, P.S. Hernandez-Montes, A. Gordillo, P. Gómez-Sal, C. López Mardomingo, E. de Jesús. Water-Soluble Palladium(II) Complexes with Sulfonated N-Heterocyclic Carbenes in Suzuki Cross-Coupling and Hydrodehalogenation Reactions. [\*Organometallics\* \*\*34\*\*, 1855–1863 \(2015\)](#). Times cited: 23. Top 20 Most Read Articles from *Organometallics* in May 2015.
7. E. A. Baquero, J. C. Flores, J. Perles, P. Gómez-Sal, E. de Jesús, Water-Soluble Mono- and Dimethyl N-Heterocyclic Carbene Platinum(II) Complexes: Synthesis and Reactivity, [\*Organometallics\*, \*\*33\*\*, 5470–5482 \(2014\)](#). Times cited: 13.
8. E. A. Baquero, S. Tricard, J. C. Flores, E. de Jesús, B. Chaudret, Highly Stable Water-Soluble Platinum Nanoparticles Stabilized by Hydrophilic N-Heterocyclic Carbenes, [\*Angew. Chem. Int. Ed.\* \*\*53\*\*, \(2014\) 13220–13224](#). Citaciones: 45. Selected as Hot-Topics of Wiley-VCH on Surfaces and Interfaces.
9. E. A. Baquero, G. F. Silbestri, P. Gómez-Sal, J. C. Flores, E. de Jesús, Sulfonated Water-soluble N-Heterocyclic Carbene Silver(I) Complexes: Behavior in Aqueous Medium and as NHC-transfer Agents to Platinum(II), [\*Organometallics\*, \*\*32\*\*, 2814–2826 \(2013\)](#). Times cited: 33. Top 10 Most Read Articles from *Organometallics* in Q2 2013.
10. A. Gordillo, M. A. Ortuño, C. López-Mardomingo, A. Lledós, G. Ujaque, E. de Jesús. Mechanistic Studies on the Pd-catalyzed Vinylation of Aryl Halides with Vinylalkoxysilanes in Water: the Effect of the Solvent and NaOH Promoter. [\*J. Am. Chem Soc.\*, \*\*135\*\*, 13749–13763 \(2013\)](#). Times cited: 25.

## C.2. Research Projects and Grants

1. N-Heterocyclic Carbene Ligands for the Preparation of Mononuclear Pd(I) Complexes and Group 10 and 11 Hydrosoluble Complexes and Nanoparticles. Ministerio de economía, industria y competitividad. Ref. CTQ2017-85203-P (80.000 €). 1/01/2018-31/12/2020. Main researcher: Dr. Ernesto de Jesús Alcañiz (IP1), Dr. Juan Carlos Flores Serrano (IP2).
2. Metal Complexes based on N-Heterocyclic Carbene Ligands: From Aqueous Chemistry to Catalyst Recovery. Ministerio de Economía y Competitividad. Ref. CTQ2014-55005-P (85.000 €). 1/01/2015-31/01/2017. Main researcher: Dr. Ernesto de Jesús Alcañiz (IP1), Dr. Juan Carlos Flores Serrano (IP2).
3. Homogeneous catalysts confined in solid supports, dendrimers or aqueous phase. Ministerio de Ciencia e Innovación. Ref. CTQ2011-24096 (111.000 €). 1/01/2012-31/12/2014. Main researcher: Dr. Ernesto de Jesús Alcañiz.

## C.3. Contracts

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## C.4. Patents and other IPR

1. F. J. Martínez Olid, R. Andrés, E. de Jesús, J. C. Flores, K. Heuzé, L. Vellutini. Complejos NHC de paladio heterogeneizados y sus usos como catalizadores recuperables. Register number: **ES 2555613 A1**. Priority date: 26/06/14. Holder entity: Universidad de Alcalá. Priority countries: España. Also published with the same authors and priority date as: **WO 2015 197890 A1**. Countries: States signing the PCT accord.
2. F. J. Martínez Olid, R. Andrés, E. de Jesús, J. C. Flores. Complejos NHC de paladio heterogeneizables. Register number: **ES 2555328 A1**. Priority date: 26/06/14. Holder entity: Universidad de Alcalá. Priority countries: España. Also published with the same authors and priority date as: **WO 2015 197891 A1**. Countries: States signing the PCT accord.

### **C.5. Invited lectures (last 5 years)**

1. Invited lectures in scientific meetings organized by chemical societies: 3
2. Invited lectures in universities, research centers and other scientific meetings: 8

### **C.6. Other**

Codirector of the Fine Chemistry Doctorate, Universidad de Alcalá, (2010–2012)

Director of the Del Rio Chemical Research Institute (Universidad de Alcalá)

Member of the Chemistry Commission of the Spanish National Agency of Prospective (ANEP) (2012-2015).