

**Personal information:** Daniel ESCUDERO (born 15<sup>th</sup> of May 1984 in Palma de Mallorca, Spain)

Researcher unique identifier(s): <http://www.researcherid.com/rid/B-9103-2008/> /  
<http://scholar.google.es/citations?hl=es&user=SPst3qEAAAAJ>

### Current Position [since november 2014]

**Postdoctoral Research Associate** at CEISAM, Université de Nantes (<http://www.sciences.univ-nantes.fr/CEISAM/>), Nantes, France)

Member of the **ModES** (Modélisation Et Spectroscopie) **team** (Prof. Denis Jacquemin)

### Research topics

1. **Computational photochemistry** and **spectroscopy** of transition-metal (TM) complexes and organic compounds: absorption, emission, non-adiabatic photochemistry.
2. Methodology: **Quantum Chemical** and **Reaction Dynamical methods**. Extensive **benchmarking** of wavefunction, Density Functional Theory (DFT) and mixed wavefunction/DFT **methods**.
3. **Photoapplications** of TM complexes in Photovoltaics (**Dye-sensitised solar cells**) and in Organic Electronics (**Organic light-emitting diodes**).
4. **Non-covalent interactions** and **cooperativity effects** among non-covalent interactions.
5. **Spin-states** in **Biochemistry**.

### Degrees

October 2011	<b>Doctor rerum naturalium (Dr. rer. nat.)</b> by the Friedrich-Schiller-Universität (FSU) Jena. Thesis title: "Spectroscopy and Photochemistry of Transition Metal Complexes: A Quantum Chemical Study". PhD supervisor: <b>Prof. Dr. Leticia González</b> . Grade: " <i>Summa Cum Laude</i> " <sup>1</sup>
July 2007	<b>Graduated</b> in Chemistry (Licenciado) by the University of the Balearic Islands (UIB), Spain. Major: Organic Physical Chemistry. Grade: 97 %
June 2002	<b>University Entrance Degree in Spain (Selectividad)</b> . Grade: 87

### Fellowships and awards

2012	<b>Green Photonics STIFT Sonderpreis Thüringen</b> PhD award. <sup>2</sup>
Aug. 2008 – Aug. 2011	<b>Carl-Zeiss Stiftung</b> PhD fellowship
Oct. 2007 - Aug. 2008	<b>Graduate scholarship</b> to extend studies abroad (Sa Nostra Foundation).
2007	Award to the <b>best graduate student in Chemistry</b> (UIB, Spain)

### Professional Positions

Nov. 2014-	<b>CEISAM, University of Nantes</b> (Prof. Denis Jacquemin)
Nov. 2011 – Nov. 2014	<b>Max-Planck-Institute for Coal Research</b> (Prof. Walter Thiel)
Oct. 2007 – Oct. 2011	<b>Institute of Physical Chemistry</b> (Prof. Leticia González), Friedrich-Schiller Universität Jena.
Oct. 2006 - Sept. 2007	<b>Dept. of Organic Chemistry</b> (Prof. Antonio Frontera and Prof. Pere M. Deyà), UIB, Spain.
July 2006 - Oct. 2006	<b>Dept. of Peptide &amp; Protein Chemistry</b> (Prof. Isabel Haro), Spanish National Research Council (CSIC), Barcelona, Spain.
Nov 2003 - Febr. 2004	<b>Dept. of Organic Chemistry</b> (Prof. Ángel García-Raso), UIB, Spain.

☞ *Working independently* since 2012, mainly on the excited-states of TM complexes.

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<sup>1</sup> Highest degree in the german education system.

<sup>2</sup> Best PhD thesis in the context of Green Photonics. Otorqued by the « Fraunhofer Innovationscluster »

### Teaching and pedagogical activities

- ✓ Computer exercises (Theoretical Chemistry CIV-VF7) at the FSU Jena during academic years 2009 and 2010.
- ✓ Responsible of Physical and Organic Chemistry practical traineeships at the FSU Jena during academic years 2008 and 2011.

### Supervision

- ✓ Supervision of seven practical traineeships at the FSU Jena (TD-DFT, Ru(II) polypyridyl dyes, Pt complexes)
- ✓ External European referee of the PhD thesis of Dr. Andre Ribeiro dos Santos (Universidad Complutense de Madrid, Spain)

### International Cooperation / Collaborative projects

- ✓ Participation in the **COST Actions CM1305** ("Explicit Control Over Spin-states in Technology and Biochemistry", **ECOSTBio**) and **CM1202** ("Supramolecular photocatalytic water splitting", **PERSPECT-H<sub>2</sub>O**)
- ✓ **International independently initiated collaborations** with Prof. Elisabeth Holder (Germany), Prof. Hans-Jørgen Aagard Jensen (Denmark), Prof. Debasis Das (India), Prof. Rainer Streubel (Germany), leading to several **joint publications**.

### Evaluation and reviewing activities

- ✓ External (German) reviewer for 1 Colombian national project (2013).
- ✓ **Reviewer of 21 articles during 2013-2014**. Since 2012, articles reviewed for: *Chem. Phys.*; *Chem. Phys. Lett.*; *Phys. Chem. Chem. Phys.*; *Inorg. Chem.*; *J. Phys. Chem.*, *J. Molec. Model.*, *Chemical Monthly*, etc.

### Scientific track-Record

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#### Bibliometric Information

- Author of **41 articles** in international peer-reviewed journals. **8 oral contributions** and **14 poster presentations** in international conferences.
- Total number of **citations > 800**.
- Hirsch (**H**) **index: 18<sup>3</sup>**
- Two co-authored review articles
- One article is the **most cited paper** in *ChemPhysChem* in the period of 2011-2012.
- **Three front cover pages**, two in *Chem. Eur. J.* and one in *Chem. Asian J.*
- Since 2013 **first and corresponding author** of **more than 60%** of the papers.

#### List of publications:

1. C. Garau, D. Quiñonero, A. Frontera, D. Escudero, P. Ballester, A. Costa and P.M. Deyà. **MP2 study of anion- $\pi$  complexes of trifluoro-s-triazine with tetrahedral and octahedral anions.** *Chem. Phys. Lett.*, 438, 104-108 (2007).
2. D. Quiñonero, A. Frontera, D. Escudero, P. Ballester, A. Costa, P.M. Deyà. **A Theoretical Study of Anion- $\pi$  Interactions in Seven-Membered Rings.** *Chem. Phys. Chem.*, 8, 1182-1187 (2007)
3. Á. García-Raso, F. Albertí, J. Fiol, A. Tasada, M. Barceló-Oliver, E. Molins, D. Escudero, A. Frontera, D. Quiñonero, P.M. Deyà. **Anion- $\pi$  interactions in bisadenine derivatives: a combined crystallographic and theoretical study.** *Inorg. Chem.*, 46, 10724-10735 (2007)

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<sup>3</sup> Data from Google Scholar by 07/2014.

4. Á. García-Raso, F. Albertí, J. Fiol, A. Tasada, M. Barceló-Oliver, E. Molins, D. Escudero, A. Frontera, D. Quiñonero, and P.M. Deyà. **A Combined Experimental and Theoretical Study of Anion- $\pi$  interactions in Bispyrimidine Salts.** *Eur. J. Org. Chem.*, Issue 35, 5821-5825 (Cover Picture) (2007)
5. D. Escudero, A. Frontera, D. Quiñonero, A. Costa, P. Ballester, P.M. Deyà. **The Induced-Polarization Energy Map: a helpful tool for predicting geometric features of Anion- $\pi$  complexes.** *J. Chem. Theory Comp.*, 3, 2098-2107 (2007)
6. D. Quiñonero, A. Frontera, D. Escudero, P. Ballester, A. Costa, P.M. Deyà. **MP2 Study of Synergistic effects between X-H/ $\pi$  (X=C,N,O) and  $\pi$ - $\pi$  interactions.** *Theor. Chem. Accounts*, 120, 385-393 (2008)
7. D. Escudero, A. Frontera, D. Quiñonero, P. M. Deyà. **On the importance of the inclusion of the basis set superposition error counterpoise correction during optimization of ion- $\pi$  complexes.** *Chem. Phys. Lett.* 455, 325-330 (2008)
8. D. Escudero, A. Frontera, D. Quiñonero, P. M. Deyà. **Interplay between cation- $\pi$  and hydrogen bonding interactions.** *Chem. Phys. Lett.* 456, 257-261 (2008)
9. D. Quiñonero, A. Frontera, D. Escudero, P. M. Deyà. **Molecular interaction potential with polarization (MIPp) study of the interplay between ion- $\pi$  and hydrogen bonding interactions.** *The Open Chemical Physics Journal*, 1, 36-41 (2008)
10. D. Escudero, A. Frontera, D. Quiñonero, P. M. Deyà. **Interplay between edge-to-face aromatic and hydrogen bonding interactions.** *J. Phys. Chem. A*, 112, 6017-6022 (2008)
11. H. Petzold, T. Weisheit, H. Görls, H. Breitzke, G. Buntkowsky, D. Escudero, L. González, W. Weigand. **Selective carbon-carbon bond cleavage of 2,2'-dibromotolane via photolysis of its appropriate (bisphosphine)Pt<sup>0</sup> complex in solid state.** *Dalton Trans.*, Issue 15, 1979-1981 (2008)
12. G. J. Mohr, H. Müller, B. Bussemer, A. Stark, T. Carofiglio, S. Trupp, R. Heuermann, T. Henkel, D. Escudero, and L. González. **Design of acidochromic dyes for facile preparation of pH sensor layers.** *Anal. Bioanal. Chem.*, 392, 1411-1418, (2008)
13. D. Escudero, A. Frontera, D. Quiñonero, P. M. Deyà. **Interplay between anion- $\pi$  and hydrogen bonding interactions.** *J. Comp. Chem.*, 30, 75-82 (2009)
14. I.A. Gural'skiy, D. Escudero, A. Frontera, P.V. Solntsev, E.B. Rusanov, A.N. Chernega, H. Krautscheid and K.V. Domasevitch. **1,2,4,5-Tetrazine: An unprecedented  $\mu_4$ -coordination that enhances ability for anion/ $\pi$  interactions.** *Dalton Trans.*, Issue 15, 2856-2864 (2009)
15. D. Escudero, C. Estarellas, A. Frontera, D. Quiñonero, P. M. Deyà. **Theoretical and Crystallographic Study of Edge-to-Face Aromatic Interactions between Pyridine Moieties and Benzene.** *Chem. Phys. Lett.*, 30, 280-285 (2009)
16. C. Biswas, M.G.B. Drew, A. Ghosh, D. Escudero and A. Frontera. **Anion/ $\pi$ , lone-pair/ $\pi$ ,  $\pi$ / $\pi$  and hydrogen bonding interactions in a coordination complex of protonated 4,4'-bipyridine: Crystal structure and theoretical studies.** *Eur. J. Inorg. Chem.*, Issue 15, 2238-2246 (2009)
17. C. Estarellas, D. Escudero, A. Frontera, D. Quiñonero, P. M. Deyà. **Theoretical ab initio study of the interplay between hydrogen bonding, cation- $\pi$  and  $\pi$ - $\pi$  interactions.** *Theor. Chem. Accounts*, 122, 325-332 (2009)

18. B. Beyer, C. Ulbricht, D. Escudero, C. Friebe, A. Winter, L. González, U. S. Schubert. **Phenyl-1H-[1,2,3]triazoles as new cyclometallating ligands for iridium(III) complexes.** *Organometallics*, 28, 5478-5488 (2009)
19. X. Lucas, C. Estarellas, D. Escudero, A. Frontera, D. Quinonero, P.M. Deyà. **Very long-range effects: cooperativity between anion- $\pi$  and hydrogen bonding interactions.** *Chem. Phys. Chem.*, 10, 2256-2264 (2009)
20. D. Escudero, X. Lucas, C. Estarellas, A. Frontera, D. Quinonero, P.M. Deyà. **Interplay between ion- $\pi$  and hydrogen bonding interactions (Review).** *Trends Phys. Chem.*, 13, 31-53 (2009)
21. D. Escudero, M. Assmann, A. Pospiech, W. Weigand, L. González. **Substituent effects on the light-induced C-C and C-Br bond activation in (bisphosphine)( $\eta$ (2)-tolane)Pt-0 complexes. A TD-DFT study.** *Phys. Chem. Chem. Phys.*, 11, 4593-4600 (2009)
22. D. Escudero, C. Estarellas, A. Frontera, D. Quinonero, P.M. Deyà. **Cooperativity effects between non-covalent interactions: Are they important for Z-DNA stability?** *Chem. Phys. Lett.*, 485, 221-225 (2010)
23. M. Kahnes, J. Richthof, H. Görls, D. Escudero, L. González, M. Westerhausen. **Mechanistic studies on the alcoholysis and aminolysis of [(MeZn)<sub>2</sub>{ $\mu$ -N(H)*t*Bu}{ $\mu$ -N(CH<sub>2</sub>Py)<sub>2</sub>}]**. *J. Organomet. Chem.*, 695, 280-290 (2010)
24. S. Hazra, B. Sarkar, M. G. B. Drew, A. Frontera, D. Escudero, A. Ghosh. **Self-assembly of coordination polymers of Cd(II), hexamine and mono-carboxylates: Structural analysis and theoretical studies of supramolecular interactions.** *Cryst. Growth Des.*, 10, 1667-1687 (2010)
25. B. Happ, D. Escudero, M.D. Hager, C. Friebe, A. Winter, H. Gørls, E. Altuntas, L. González, U.S. Schubert. **N-heterocyclic donor- and acceptor-type ligands based on 2-(1H-[1,2,3]triazol-4-yl)pyridines and their ruthenium(II) complexes.** *J. Org. Chem.* 75, 4025-4038 (2010)
26. N. Tian, D. Lenkeit, S. Pelz, L.H. Fischer, D. Escudero, R. Schlewke, D. Klink, O. J. Schmitz, L. González, M. Schäferling, E. Holder. **Structure-property relationship of red- and green-emitting iridium(III) complexes with respect to their temperature and oxygen sensitivity.** *Eur. J. Inorg. Chem.* 4875-4885 (2010)
27. T. Weisheit, D. Escudero, H. Petzold, H. Görls, L. González, W. Weigand. **Photochemical behaviour of (bisphosphine)( $\eta$ (2)-tolane)Pt-0 complexes in solution and in the solid state. Part A: Experimental considerations.** *Dalton Trans.*, 39, 9493-9504 (2010)
28. D. Escudero, T. Weisheit, W. Weigand, L. González. **Photochemical behaviour of (bisphosphine)( $\eta$ (2)-tolane)Pt-0 complexes in solution and in the solid state. Part B: An insight from DFT calculations.** *Dalton Trans.*, 39, 9505-9513 (2010)
29. B. Schulze, D. Escudero, C. Friebe, R. Siebert, H. Görls, U. Köhn, E. Altuntas, A. Baumgärtel, M. D. Hager, A. Winter, B. Dietzek, L. González, U.S. Schubert. **Long excited state lifetime and strong room temperature phosphorescence of a heteroleptic bis-tridentate ruthenium(II) complex: A pincer-ligand with click-derived triazolynes as superior donors.** *Chem. Eur. J.*, 11, 5494-5498 (*Back Cover*) (2011)
30. D. Escudero, S. Trupp, B. Bussemer, G. Mohr, L. González. **Spectroscopic properties of azobenzene-based pH indicator dyes: a quantum chemical and experimental study.** *J. Chem. Theory Comp.*, 7, 1062-1072 (2011)
31. L. González, D. Escudero, L. Serrano-Andrés. **Progress and challenges in the calculation of electronic excited states. (Review)** *ChemPhys Chem.* 13, 28 (2012)

32. D. Escudero, L. González. **RASPT2/RASSCF vs range-separated/hybrid DFT methods: assessing the excited states of a Ru(II)bipyridyl complex.** *J. Chem. Theory Comp.* 8, 203 (2012)
33. D. Escudero, B. Happ, A. Winter, M. D. Hager, U. S. Schubert, L. González. **The radiative decay rates tune the emissive properties of Ru(II) polypyridyl complexes. A computational study.** *Chem. Asian J.* 7, 4 (**Back cover**) (2012)
34. B. Schulze, D. Escudero, C. Friebe, R. Siebert, H. Görls, S. Sinn, M. Thomas, S. Mai, J. Popp, B. Dietzek, L. González, U. S. Schubert. **Ruthenium(II) photosensitizers of tridentate click-derived cyclometalating ligands: a joint experimental and computational study.** *Chem. Eur. J.*, 18, 13 (2012)
35. R. Goy, U.-P. Apfel, C. Elleouet, D. Escudero, M. Elstner, H. Görls, J. Talarmin, P. Schollhammer, L. González, W. Weigand. **A silicon-heteroaromatic system as photosensitizer for light-driven hydrogen production by hydrogenase mimics.** *Eur. J. Inorg. Chem.*, 4466 (2013)
36. D. Escudero, E. Heuser, R. J. Meier, M. Schäferling, W. Thiel, E. Holder. **Unveiling photodeactivation pathways for a new iridium(III) cyclometalated complex.** *Chem. Eur. J.*, 19, 15639, (2013)
37. D. Escudero, A. Frontera, R. Streubel. **Electronic structure of N<sub>2</sub>P<sub>2</sub> four-membered rings.** *ChemPhysChem*, 15, 1599 (2014)
38. D. Escudero, W. Thiel. **Assessing the density functional theory-based multireference interaction (DFT/MRCI) method for transition metal complexes.** *J. Chem. Phys.*, 140, 194105 (2014)
39. D. Das, P. Chakraborty, J. Adhikary, S. Samanta, D. Escudero, A. C. Castro, M. Swart, A. Frontera, A. Bauza, S. Ghosh, E. Zangrando. **A combined experimental and theoretical investigation on ligand and anion controlled complex formation with unprecedented structural features and photoluminescence properties of Zn(II) complexes.** *Crystal Growth & Design*, DOI:10.1021/cg500717n (2014)
40. D. Escudero, W. Thiel. **Exploring the triplet excited state potential energy surfaces of a cyclometalated Pt(II) complex: Is there Non-Kasha emissive behavior?** *Inorg. Chem.*, 53, 11015 (2014)
41. S. Holle, D. Escudero, B. Inés, J. Rust, W. Thiel, M. Alcarazo. **On the Reactivity of Tetrakis(trifluoromethyl)cyclopentadienone towards Carbon-based Lewis Bases.** *Chem. Eur. J.*, Accepted (2014)

#### Significant invited oral plenary contributions:

- ✓ *Multi-determinantal-based DFT studies of the excited states of TM complexes*, ESCMQC14, (Houffalize, Belgium, 10 September 2014).
- ✓ *Computational studies on photoactive materials*, Faculty Position Interview (UCL, Louvain-la-Neuve, Belgium, 25 February 2014).
- ✓ *Computational studies on photoactive materials*, Faculty Position Interview (KU Leuven, Belgium, 4 December 2013).

#### Other merits:

- ✓ Member of the management board of the “Sociedad CERFA” (Society of Spanish Researchers in the Bundesrepublik Deutschland)
- ✓ Co-organizer of the first symposium of the “Sociedad CERFA”: Passion for Knowledge: Bridging Spanish-German cooperation in R&D (Cologne, 28 March 2014).