

Curriculum Vitæ

1 Personal information



Name: IÑAKI SILANES CRISTÓBAL

Birth date: June 11, 1977

Address: Oriako Pasealekua 36, 2nd C, 20200 Beasain (Gipuzkoa)

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2 Academic training

- **Ph.D.:** Computational Chemistry (2006)
Title: *Ethylene Polymerization by Group IV Transition Metal Metallocenes*
Center: UPV-EHU Chemistry Faculty at Donostia
Areas of knowledge: Quantum Chemistry, Physical Chemistry
Doctoral program: Theoretical and Computational Chemistry
Courses taken:
“Inter-university doctoral course on Theoretical and Computational Chemistry”
Valencia, Spain, January 22 - February 17, 2001
- **University Degree:** Chemistry (2000)
Center: UPV-EHU Chemistry Faculty at Donostia
Area of knowledge: Macromolecular Chemistry

3 Present professional situation

- **Position:** Post-doctoral fellow
Organization: Donostia International Physics Center (DIPC)
Supervisor: Andrés Arnau
Telephone: 943 015341
Fax: 943 015270

4 Former scientific activities

- **Position:** Research group member
Organization: UPV-EHU
Period: Jan-Dec 2006
Department: Polymer Science and Technology
Group head: Jesus M. Ugalde
- **Position:** Project-bound scholar
Organization: UPV-EHU
Project: Bottom-up approximation in nanotechnology. Two examples: nanospheres and monodimensional nanowires.
Period: May-December, 2005

Department: Polymer Science and Technology
Director: Jesus M. Ugalde

- **Position:** Pre-doctoral scholar
Organization: Basque Government - Eusko Jaurlaritza
Period: 2000-2004
Thesis director: Jesus M. Ugalde
- **Position:** Collaboration scholar
Organization: UPV-EHU Chemistry Faculty at Donostia
Period: 1998-2000
Supervisor: Jesus M. Ugalde

5 Languages

Spanish: Native.
Basque: Native. *Euskararen Gaitasun Agiria* (EGA)
English: High level. *Cambridge Advanced Exam* (CAE)

6 Supported research projects

- **Title:** "Transition metal clusters. Electronic screening"
Supporting organization: UPV-EHU
Period: 1998-2000
Main researcher: Jesus M. Ugalde

7 Publications

1. "Spectroscopic fingerprints of amine and imide functional groups in self-assembled monolayers"
M. Ruiz-Osés, T. Kampen, N. González-Lakunza, I. Silanes, P.M. Schmidt-Weber, A. Gourdon, A. Arnau, K. Horn, J.E. Ortega
ChemPhysChem **2007**, *8(11)*, 1722–1726
2. "Counterintuitive effects of the electron correlation in the first excited $^1\Sigma_g^+$ state of the hydrogen molecule"
J. Wang, J.M. Mercero, I. Silanes and J. M. Ugalde
Europhysics Letters **2006**, *76(5)*, 808–814
3. "Self-assembly of heterogeneous supramolecular structures with uniaxial anisotropy"
M. Ruiz-Osés, N. González-Lakunza, I. Silanes, A. Gourdon, A. Arnau and J.E. Ortega
J. Phys. Chem. B **2006**, *110(51)*, 25573–25577
4. "Comparison of Ti, Zr and Hf as cations for metallocene-catalyzed olefin polymerization"
I. Silanes, J.M. Mercero and J. M. Ugalde
Organometallics **2006**, *25(19)*, 4483–4490
5. "A joint experimental and theoretical study of cation- π interactions: Multiple-decker sandwich complexes of ferrocene with alkali metal ions (Li^+ , Na^+ , Rb^+ , Cs^+)"
A.H. Ilkhechi, J.M. Mercero, I. Silanes, M. Bolte, M. Scheibitz, H-W. Lerner, J.M. Ugalde and M. Wagner
J. Am. Chem. Soc. **2005**, *127*, 10656–10666

6. "Comparative study of various mechanisms for metallocene-catalyzed α -olefin polymerization"
I. Silanes and J.M. Ugalde
Organometallics, **2005**, *24(13)*, 3233–3246.
7. "Minimal dipole charge for a dipole-bound dianion"
I. Silanes, H.J.J. van Dam and J.M. Ugalde
Mol. Phys. **2003**, *101*, 2529–2532
8. "Electron correlation studies by means of electron-pair density functions"
E. Valderrama, X. Fradera, I. Silanes, J.M. Ugalde and R.J. Boyd
Reviews in Modern Quantum Chemistry: A celebration of the contributions of Robert G. Parr. Ed. K.D. Sen, World Scientific, Singapore, **2002**
9. "Atomic charge states in a weakly coupled plasma environment"
I. Silanes and J. M. Mercero and J.M. Ugalde
Phys. Rev. E **2002**, *66*, 026408
10. "The ferrocene-lithium cation complex in the gas phase"
A. Irigoras, J.M. Mercero, I. Silanes and J. M. Ugalde
J. Am. Chem. Soc. **2002**, *123*, 5040–5043
11. "Cusp conditions for non-Coulombic interactions"
I. Silanes, J.M. Ugalde and R.J. Boyd
J. Mol. Struct. (Theochem) **2000**, *527*, 27–33
12. "Reactivity of $\text{Co}^+(\text{}^3\text{F}, \text{}^5\text{F})$, $\text{Ni}^+(\text{}^2\text{D}, \text{}^4\text{F})$, and $\text{Cu}^+(\text{}^1\text{S}, \text{}^3\text{D})$: reaction of Co^+ , Ni^+ and Cu^+ with water"
A. Irigoras, O. Elizalde, I. Silanes, J.E. Fowler and J.M. Ugalde
J. Am. Chem. Soc. **2000**, *122(1)*, 114–122

8 International congresses

8.1 Talks

- Nanotron 2007
"Molecular self-assembly for nanoscale electronics"
Donostia (Spain), May 10, 2007

8.2 Posters

- TNT2007: Trends in NanoTechnology
"Self-assembly of $\text{NC-Ph}_3\text{-CN}$ molecules on $\text{Ag}(111)$: Formation of 2D hydrogen-bonded and metal-organic networks"
Donostia (Spain), September 3–7, 2007
- ESPA2006. Electronic Structure: Principles and Applications
"Comparison of Ti , Zr and Hf as cations for metallocene-catalyzed olefin polymerization"
Santiago de Compostela (Spain), July 18–21, 2006
- 3rd NanoSpain Workshop
"Supramolecular self-assembly on flat and vicinal $\text{Au}(111)$ "
Pamplona (Spain), March 20–23, 2006
- TeoBio-05. Theoretical Biophysics Symposium
"Formation of C-C bonds in the coordination sphere of Zirconium"
Örebro (Sweden), June 29–July 1, 2005

- ESPA2004. Electronic Structure: Principles and Applications
“*Pitfalls of the Cossée-Arlman mechanism for olefin polymerization*”
Valladolid (Spain), September 15–17, 2004
- ESPA2002. Electronic Structure: Principles and Applications
“*Critical Conditions for true Dipole-Bound Dianions*”
Sevilla (Spain), September 11–13, 2002
- Electron densities and electron distributions workshop
“*Cusp conditions for non-Coulombic interactions*”
Donostia (Spain), April 27–28, 2000

8.3 Assistance

- SMS2006. Spanish Molecular Electronics Symposium.
Donostia (Spain), March 24, 2006
- Albert Einstein’s *Annus Mirabilis* Congress
Donostia (Spain), September 5–8, 2005
- Theoretical Biophysics Symposium
Donostia (Spain), March 5–7, 2003
- One Day Workshop On Physical Chemistry
Donostia (Spain), July 5, 2001
- ESPA2000. Electronic Structure: Prediction and Applications
Donostia (Spain), October 4–6, 2000

9 Stays in foreign centers

- **Center:** CCLRC Daresbury Laboratory, Daresbury (UK)
Starting date: September 2001
Duration: 13 weeks
Subject: Acquisition of expertise in the use of Quantum Chemistry software

10 Computer science

- User-level knowledge on **Windows** and **Unix** platforms, and system administrator level experience in **Linux** environments.
- **Programming:** Perl, C-shell, HTML, CSS, L^AT_EX, Fortran, PHP, Python
- Utility programs:
 - **Quantum calculation** (Gaussian, SIESTA, GAMESS)
 - **Office related** (OpenOffice, KOffice, MS Office)
 - **2D and 3D data plotting** (Grace, GNUPlot)
 - **Calculus and algebra** (Mathematica)
 - **Web development** (Quanta+, Bluefish, Macromedia Flash)
 - **Manipulation of 2D images** (GIMP, Photoshop)
 - **Firewalling** (Firestarter, Guarddog)
- **Practical Computing For Scientists** course (50h), DIPC (2001)

- **Web page animation with Flash** course (18h), Aula Gaztekutxa (2005)
- **Image manipulation with Photoshop** course (12h), Aula Gaztekutxa (2004)
- **Computer hardware workshop** course (12h), Aula Gaztekutxa (2004)

11 Teaching experience

- Substitution in 3rd course *Physical Chemistry* (theory, 2005)
- Substitution in 5th course *Physical Chemistry* (computer practice, 2005-2006)

12 Other

- **B1 driving license**
- *Kutxa Fin de Carrera* prize for my Degree (2000)
- *Premio Extraordinario de Bachillerato* price at High school (1995)
- Guide in the yearly *Open Doors Days*, taking place at the UPV-EHU Chemistry Faculty at Donostia (2002-2005)
- **Norma ISO 14000** course (20h), UPV-EHU Chemistry Faculty at Donostia (2002)
- **Photography** course (14 h), Aula Gaztekutxa (2003)
- **Photographic improvement** course (14h), Aula Gaztekutxa (2004)
- 2500+ editions in Wikipedia (User:Isilanes)