

Julia Contreras-García

PERSONAL DATA

Date of birth : 24/05/1980 **Gender:** F
Nationality: Spanish
Postal Address:
Facultad de Químicas
Department: Physical and analytical chemistry
Address: C/Julián Clavería sn, Oviedo, Spain
E-mail Address: julia@carbono.quimica.uniovi.es
Telephone: 0034985102991
Fax: 0034985103125

ACADEMIC BACKGROUND

General Studies	Centre	Dates
Bachelor	IES Monte Naranco (Extraordinarity Award)	1994-1997
Access to University	IES Monte Naranco (Matrícula de Honor)	1998
Chemistry	Universidad de Oviedo (Best graduated 2003)	1998-2003
Project in Chemistry	U. de Oviedo (Extraordinarity Award) North London University (Excellence in Erasmus)	2004
Diploma Superior de Inglés	EOI de Oviedo	2003
Diploma Superior de Francés	EOI de Oviedo	2003
Diploma Medio de Alemán	EOI de Oviedo	2007

M.B.A.	Centre	Dates
Química Teórica y Computacional	Universidad de Oviedo (Sobresaliente)	2004-2005

PhD	Centre	Dates
Química Teórica y Computacional	Universidad de Oviedo (Sobresaliente cum Laude)	2005-2009

Scientific jobs

Job	Centre	Dates
Postdoctoral researcher	Universidad de Oviedo	2008-2009
Scientific translator	Universidad de Oviedo	2004

LANGUAGES (N = NORMAL, G = GOOD, P = PERFECTLY)

<i>Language</i>	<i>Speaking</i>	<i>Reading</i>	<i>Writing</i>
<i>English</i>	<i>P</i>	<i>P</i>	<i>P</i>
<i>French</i>	<i>P</i>	<i>P</i>	<i>P</i>
<i>German</i>	<i>N</i>	<i>N</i>	<i>N</i>
<i>Italian</i>	<i>N</i>	<i>N</i>	<i>N</i>

Invited Talks

TITLE: Caminos de transición, vibraciones cristalinas
CONGRESS: IIEAP
MEETING PLACE: Barcelona, Spain
YEAR: 2007

TITLE: From molecular to polymeric CO₂: understanding bonding transformations under pressure
CONGRESS: EHPRG
MEETING PLACE: Valencia, Spain
YEAR: 2008

Invited Chairperson

TITLE: Molecular crystals under pressure: Experiments and Theory (Microsymposium)
CONGRESS: EHPRG
MEETING PLACE: Valencia, Spain
YEAR: 2008

Stays at Internationally Recognized Centres

CENTRE: Université Pierre et Marie

PLACE: Paris

COUNTRY: France

YEAR: 2005

LENGTH: 11 weeks

TOPIC: Implementation of the topological analysis of the electron localization function in crystalline solids

CENTRE: ETH-Zürich

PLACE: Zürich

COUNTRY: Switzerland

YEAR: 2007

LENGTH: 12 weeks

TOPIC: Study of the anion in metallic matrices model by means of ELF

Publications in Books

Authors: J. Contreras-García, B. Silvi, J. M. Recio

Chapter Title: How ELF quantifies and pictures bonding changes along phase transitions (invited)

Book: Modern Charge Density Analysis (in elaboration)

Publications in Journals

Authors: J. Contreras-García, A. M. Pendás, B. Silvi, J. M. Recio

Title: Useful Applications of the Electron Localization Function in High Pressure Crystal Chemistry

Journal: J. of Phys. Chem. Solids 69, 2204 (2008)

Authors: M. Marqués, J. Contreras-García, M. Flórez, J. M. Recio

Title: On the mechanism of the zircon-reidite pressure induced transformation

Journal: J. Phys. Chem. Solids 69, 2277 (2008)

Authors: J. Contreras-García, A. M. Pendás, J. M. Recio

Title: How ELF quantifies and pictures chemical changes in a solid: the B3-B1 pressure induced phase transition in BeO

Journal: J. Phys. Chem. B. 112, 9787 (2008)

Authors: G. J. Ackland, M. Marqués, J. Contreras-García, M. I. McMahon

Title: Total energy calculations of high pressure phosphorous: the origin of incommensurate modulations in P-IV

Journal: Phys. Rev. B 78, 054120 (2008)

NOTE: Editor's suggestion

Authors: J. Contreras-García, A. M. Pendás, B. Silvi, J. M. Recio

Title: Bases for Understanding Polymerization under Pressure: The Practical Case of CO₂

Journal: J. Phys. Chem. B., 113, 1068 (2009)

Authors: N. Barrier, J. M. Rueff, M. B. Lepetit, J. Contreras-García, S. Malo, B. Raveau

Title: A new polymorph with a layered structure ϵ -CaTe₂O₅

Journal: Solid State Sciences, 11, 289 (2009)

Authors: J. Contreras-García, A. M. Pendás, B. Silvi, J. M. Recio

Title: Computation of local and global properties of the ELF topology in crystals

Journal: J. Theor. Chem. Comp. 113, 1068 (2009)

Authors: M. Flórez, M. Marqués, J. Contreras-García, J. M. Recio

Title: Quantum mechanical calculations of zircon-reidite transition pathways in ZrSiO₄

Journal: Phys. Rev. B (accepted)

Authors: J. Contreras-García, J. M. Recio

Title: From molecular to polymeric CO₂: bonding transformations under pressure

Journal: High Press. Res. (accepted)

Authors: L. Gracia, J. Contreras-García, A. Beltrán, J. M. Recio

Title: Bonding changes across the α -cristobalite \rightarrow stishovite transition path

Journal: High Press. Res. (accepted)

Authors: A. Waskowska, L. Gerward, J. Staun Olsen, M. Marqués, J. Contreras-García, J. M. Recio
Title: The bulk modulus of cubic spinel selenides: An experimental and theoretical study

Journal: High Press. Res. (accepted)

Authors: M. Taravillo, E. del Corro, J. Contreras-García, A. M. Pendás, M. Flórez, J. M. Recio, and V. G. Baonza
Title: Universal compressibility behaviour of ions in ionic crystals

Journal: High Press. Res. (accepted)

Authors: J. Contreras-García, P. Mori-Sánchez, B. Silvi, J. M. Recio
Title: Towards a quantum-chemical interpretation of compressibility in solids

Journal: J. Phys. Chem. B (submitted)

Authors: J. Contreras-García, J. M. Recio
Title: Properties of alkali halides from their VSEPR structure

Journal: (to be published)

Authors: J. Contreras-García, P. Mori-Sánchez, J. M. Recio
Title: Compressibility of covalent solids from combined Bond Charge Model and Electron Localization studies

Journal: (to be published)

Presentations In Congresses

AUTHORS: J. Contreras-García, M. Marqués, M. Flórez, J. M. Recio
TITLE: Thermodynamic and mechanistic aspects of the pressure induced transformation sequence in AgCl
TYPE OF PRESENTATION: *Poster*
CONGRESS: *ESPA04*
MEETING PLACE: *Valladolid, Spain*
YEAR: *2004*

AUTHORS: J. Contreras-García, M. Marqués, M. Flórez, J. M. Recio
TITLE: Aspectos termodinámicos y mecanísticos de las transiciones inducidas por presión en el AgCl
TYPE OF PRESENTATION: *Oral*
CONGRESS: *IIEAP*
MEETING PLACE: *Madrid, Spain*
YEAR: *2004*

AUTHORS: J. Contreras-García, M. Marqués, M. Flórez, J. M. Recio
TITLE: The symmetry underlying the pressure-induced polymorphism in AgCl
TYPE OF PRESENTATION: *Poster*
CONGRESS: *International School of Mathematical and Theoretical Crystallography*
MEETING PLACE: *Nancy, France*
YEAR: *2005*

AUTHORS: J. Contreras-García, M. Marqués, M. Flórez, J. M. Recio
TITLE: Aspectos Quantum mechanical simulation of pressure induced polymorphism in AgCl
TYPE OF PRESENTATION: *Oral*
CONGRESS: *20th AIRAPT-43rd EHPRG*
MEETING PLACE: *Karlsruhe, Germany*
YEAR: *2005*

AUTHORS: J. Contreras-García, A. M. Pendás, J. M. Recio
TITLE: Automated análisis of the topology of the electron localization function (ELF) in crystals
TYPE OF PRESENTATION: *Poster*
CONGRESS: *ESPA06*
MEETING PLACE: *Santiago de Compostela, Spain*
YEAR: *2006*

AUTHORS: J. Contreras-García, A. M. Pendás, B. Silvi, J. M. Recio
TITLE: Implementation of the análisis of ELF-topology in crystals
TYPE OF PRESENTATION: Poster
CONGRESS: Faraday Discussions 135
MEETING PLACE: Manchester, UK
YEAR: 2006

AUTHORS: M. Marqués, J. Contreras-García, M. Flórez, J. M. Recio
TITLE: Breakdown of a displacive conception in the zircon-reidite transformation
TYPE OF PRESENTATION: Poster
CONGRESS: Study of Matter at Extreme Conditions (SMEC07)
MEETING PLACE: Miami
YEAR: 2007

AUTHORS: J. Contreras García
TITLE: Camino de transición, vibraciones cristalinas
TYPE OF PRESENTATION: Oral
CONGRESS: III Escuela de Altas Presiones (III EAP)
MEETING PLACE: Barcelona
YEAR: 2007

AUTHORS: G. J. Ackland, M. Marqués, J. Contreras-García, M. McMahon
TITLE: Total energy calculations of high pressure phosphorous: the origin of incommensurate modulations in P-IV
TYPE OF PRESENTATION: Poster
CONGRESS: Workshop on Advances in High Pressure Crystallography at Large Scale Facilities
MEETING PLACE: Oxford
YEAR: 2007

AUTHORS: J. Contreras-García, J. M. Recio
TITLE: Deeper understanding of molecular solids under pressure
TYPE OF PRESENTATION: Poster
CONGRESS: Electron Localizability and chemical bonding (ELI08)
MEETING PLACE: Dresden
YEAR: 2008

AUTHORS: J. Contreras-García, A. M. Pendás, B. Silvi , J. M. Recio
TITLE: Understanding and quantifying polymerization in CO₂
TYPE OF PRESENTATION: Poster
CONGRESS: 5th-European Charge Density Meeting-DFG1178
MEETING PLACE: Gravedona, Italy
YEAR: 2008

AUTHORS: J. Contreras-García
TITLE: From molecular to polymeric CO₂: understanding bonding transformations under pressure
TYPE OF PRESENTATION: Oral
CONGRESS: EHPRG
MEETING PLACE: Valencia, Spain
YEAR: 2008

AUTHORS: M. Taravillo, E. del Corro, J. Contreras-García, M. Flórez, J. M. Recio, V. G. Baonza
TITLE: Universal compressibility behaviour of ions in ionic crystals
TYPE OF PRESENTATION: Poster
CONGRESS: EHPRG
MEETING PLACE: Valencia, Spain
YEAR: 2008

AUTHORS: M. Flórez, M. Marqués, J. Contreras-García, J. M. Recio
TITLE: Structural, energetic and bonding changes across transition pathways: Application to some oxide crystals
TYPE OF PRESENTATION: Poster
CONGRESS: EHPRG
MEETING PLACE: Valencia, Spain
YEAR: 2008

AUTHORS: L. Gracia, J. Contreras-García, A. Beltrán, J. M. Recio
TITLE: Bonding changes across the α -cristobalite \rightarrow stishovite transition path
TYPE OF PRESENTATION: Poster
CONGRESS: EHPRG
MEETING PLACE: Valencia, Spain
YEAR: 2008

AUTHORS: E. Beret, J. Contreras-García
TITLE: Electron localizability and preferential solvation sites
TYPE OF PRESENTATION: Poster
CONGRESS: Electron Localizability and chemical bonding (ELI09)
MEETING PLACE: Dresden
YEAR: 2009

Other achievements

AWARDS

PREMIO EXTRAORDINARIO DE BACHILLERATO DE ASTURIAS (1999)

Extraordinary award among A+ students at college.

EXCELLENCE EN ERASMUS (2002)

Congratulations from Metropolitan University since all grades were A

BEST GRADUATED ON YEAR 2003

Award for being the best graduated in chemistry on year 2003 in the University of Oviedo

PREMIO EXTRAORDINARIO DE LICENCIATURA DE QUÍMICAS, U. DE OVIEDO (2004)

Best project graduated with project in chemistry on year 2004 in the University of Oviedo

FELLOWSHIPS

MATRÍCULA DE HONOR (1998)

Free university studies for some A+ students

ERASMUS FELLOWSHIP (2001)

Grant for university students to study abroad

LECTURER FORMATION FELLOWSHIP (2004)

PhD grant from the Ministry of Education

ENDING THESIS GRANT (2008)

Grant for ending outstanding thesis at Universidad de Oviedo

HPC-EUROPA FELLOWSHIP (2009)

Funding for a research visit at Pierre et Marie University (Paris)