



Carlos Vega de las Heras

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Date of document: 24/02/2025

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Summary of CV

This section describes briefly a summary of your career in science, academic and research; the main scientific and technological achievements and goals in your line of research in the medium -and long- term. It also includes other important aspects or peculiarities.

Short CV

Place/date birth: Madrid, 28th August, 1964

Bachelor degree in Chemistry (Universidad Complutense de Madrid) : 1987

PhD degree in Chemistry (Universidad Complutense de Madrid) : 1991

Fulbright post-doctoral fellow (University of Massachusetts, Amherst) : 1991, 1992

Assistant Professor (Universidad Complutense de Madrid) : 1993-1995

Associate Professor (Universidad Complutense de Madrid) : 1995-2005

Full Professor of Physical Chemistry since April 2005 (Catedrático de Química)

Research ID : C-5455-2009 (258 artículos , 18300 citas según el WOS, 23700 según Google Scholar)

Research ID: C-5455-2009 (258 papers , 18300 citations according to WOS . 23700 from Google Scholar)

h index 63 (WOS) h index 70 (Google Scholar)

Google Scholar profile : <https://scholar.google.es/citations?user=SI1Z18sAAAAJ&hl=en>

Premio Extraordinario de Licenciatura(UCM).Premio Extraordinario de Doctorado(UCM)

First Prize for the Bachelor degree and for the PhD degree in Chemistry awarded by Universidad Complutense de Madrid

Primer Premio Nacional de Licenciatura en Ciencias Químicas



First National Prize for the Bachelor degree in Chemistry in Spain (1987)

Molecular Physics Lecturer award (in recognition of an outstanding contribution to the field) , Thermodynamic Conference of the Royal Society of Chemistry (UK) .

Beca post-doctoral Fulbright 1991 and 1992

Postdoctoral Fulbright Fellow in the United States 1991 and 1992

6 sexenios de investigación , 6 quinquenios docentes

30 years of research : positive evaluation. 30 years of teaching : positive evaluation.

Estoy situado entre los primeros 1000 investigadores españoles de todas las áreas de conocimiento

(ver detalles en www.webometrics.info/en/GoogleScholar/Spain)

I am in the list of best 1000 Spanish researchers (working abroad or in Spain)

(see details in www.webometrics.info/en/GoogleScholar/Spain)

Científico seleccionado para la presentación de nominaciones al Premio Nobel de Química en los años 2013 y 2017.

I was selected to nominate candidates for the Nobel Prize in Chemistry in the years 2013 and 2017.

He formado parte de tribunales de tesis en 38 ocasiones.

I have been in PhD committees 30 times (Spain) and 8 (abroad) .

Nueve tesis doctorales dirigidas (una más en curso) .

Nine PhD students. (one more underway) . The first two are now full professors.

Luis González MacDowell (2000) , Eduardo Sanz García (2006), Maria Martín Conde (2011), Juan Luis Aragonés (2012), Jorge Reñe Espinosa (2018),

Pablo Rosales Peláez (2020), Pablo Montero de Hijos (2021), Cintia Pulido Lamas (2024), Samuel Blazquez (2024)

Editor asociado del Journal of Chemical Physics

Associate Editor of the Journal of Chemical Physics (American Institute of Physics) since 2014

Miembro del Advisory Board de la Revista Molecular Physics (Taylor and Francis)

Member of the Advisory Board of the Journal : Molecular Physics since 2010

**C****V****n**

CURRÍCULUM VITAE NORMALIZADO

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Past-post-docts in my group : Carl McBride (Marie Curie), Eva G. Noya , Chantal Valeriani , Ivan M. Zeron, Valentino Bianco (Marie Curie) , Joanna Grabowska

**C****V****N**

CURRÍCULUM VÍTAE NORMALIZADO

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Leadership Merits

Brief presentation of the merits related to leadership activities of special relevance.



General quality indicators of scientific research

This section describes briefly the main quality indicators of scientific production (periods of research activity, experience in supervising doctoral theses, total citations, articles in journals of the first quartile, H index...). It also includes other important aspects or peculiarities.

English

WOS h index 63 18300 citations 258 papers 38
papers with more than 100 citations

Google Scholar h index 70 23700 citations 258 papers 45 papers
with more than 100 citations

Research ID : C-5455-2009

9 thesis (2000,2006,2011,2012,2018,2020,2021,2024,2024). 1 more underway
(2026) .

Papers published in the period 2016-2023: 50

Citations received a year (according to Google Scholar)

2017: 1149

2018: 1565

2019: 1575

2020: 1494

2021: 1679

2022: 1762

2023: 2072

2024: 2280



Three most cited works (Google scholar)

J.L.F.Abascal y C.Vega, J.Chem.Phys., 123, 234505, (2005) : 4110 citations

J.L.F.Abascal, E.Sanz, R.G.Fernandez y C. Vega, J.Chem.Phys.,122,234511,(2005): 1533 citations

C.Vega, y J.L.F. Abascal, Physical Chemistry Chemical Physics, 13, 19663,(2011): 1041 citations

Spanish

WOS Indice H 63 , 18300 citas , 258 publicaciones , 38 artículos con más de 100 citas

Google scholar

Indice H 70 , 23700 citas , 258 publicaciones, 45 artículos con mas de 100 citas.

Research ID : C-5455-2009

9 tesis doctorales dirigidas (2000,2006,2011,2012,2018,2020,2021,2024,2024). 1 tesis doctoral más en curso (2026). 5 sexenios de investigación. 6 quinquenios docentes.

Número de citas recibidas (según Google Scholar)

2017: 1149

2018: 1565

2019: 1575

2020: 1494

2021: 1679

2022: 1762



2023: 2072

2024: 2280

Los tres trabajos más citados (según Google Scholar):

J.L.F.Abascal y C.Vega, J.Chem.Phys., 123, 234505, (2005) : 4110 citations

J.L.F.Abascal, E.Sanz, R.G.Fernandez y C. Vega, J.Chem.Phys.,122,234511,(2005):
1533 citations

C.Vega, y J.L.F. Abascal, Physical Chemistry Chemical Physics, 13, 19663,(2011):
1041 citations

Artículos publicados en el periodo 2016-2025: 84

Carlos Vega de las Heras

Surname(s): **Vega de las Heras**
Name: **Carlos**
ORCID: **0000-0002-2417-9645**
ScopusID: **8986819600**
ResearcherID: **C-5455-2009**
Date of birth: **28/08/1964**
Gender: **Male**
Personal web page: **catalan.quim.ucm.es**

Current professional situation

Employing entity: Universidad Complutense de Madrid **Type of entity:** University
Department: QUIMICA FISICA I, Facultad de Ciencias Químicas
Professional category: Catedrático de Universidad **Leadership and management (Y/N):** No
City employing entity: MADRID, Community of Madrid, Spain
Start date: 02/04/2005
Type of contract: Civil servant **Dedication regime:** Full time
Primary (UNESCO code): 230700 - Physical chemistry
Secondary (UNESCO code): 220600 - Molecular physics
Tertiary (UNESCO code): 221300 - Thermodynamics
Performed tasks: Catedrático de Universidad
Identify key words: Numerical simulation

Previous positions and activities

	Employing entity	Professional category	Start date
1	Universidad Complutense de Madrid	PROFESOR TITULAR DE UNIVERSIDAD	08/03/1995
2	Universidad Complutense de Madrid	AYUDANTE DE FACULTAD	10/10/1990
3	Universidad Complutense de Madrid	BECARIO DE FPU	01/01/1988

- 1** **Employing entity:** Universidad Complutense de Madrid
Professional category: PROFESOR TITULAR DE UNIVERSIDAD **Leadership and management (Y/N):** No
Start-End date: 08/03/1995 - 02/04/2005 **Duration:** 10 years - 28 days
Type of contract: Civil servant
Performed tasks: PROFESOR TITULAR DE UNIVERSIDAD
- 2** **Employing entity:** Universidad Complutense de Madrid
Professional category: AYUDANTE DE FACULTAD **Leadership and management (Y/N):** No



Start-End date: 10/10/1990 - 08/05/1995
Performed tasks: AYUDANTE DE FACULTAD

Duration: 4 years - 7 months - 1 day

3 Employing entity: Universidad Complutense de Madrid

Professional category: BECARIO DE FPU

Leadership and management (Y/N): No

Start-End date: 01/01/1988 - 10/10/1990

Duration: 2 years - 9 months - 13 days

Performed tasks: BECARIO DE FPU



Education

University education

1st and 2nd cycle studies and pre-Bologna degrees

Name of qualification: Licenciado en Ciencias Químicas

Degree awarding entity: Universidad Complutense de Madrid **Type of entity:** University

Date of qualification: 15/07/1987

Doctorates

Doctorate programme: Doctor en Ciencias Químicas

Degree awarding entity: Universidad Complutense de Madrid **Type of entity:** University

City degree awarding entity: Spain

Date of degree: 20/03/1991

Thesis title: Termodinámica Estadística del Estado Líquido

Obtained qualification: Sobresaliente cum laude y premio extraordinario

Language skills

Language	Listening skills	Reading skills	Spoken interaction	Speaking skills	Writing skills
French		C1	C1	C1	C1
English		C1	C1	C1	C1

Teaching experience

Experience supervising doctoral thesis and/or final year projects

- Project title:** Simulación molecular de disoluciones de electrolitos e hidratos de gas

Type of project: Doctoral thesis

Co-director of thesis: Conde M.M.; Vega C

Entity: Universidad Complutense de Madrid **Type of entity:** University

Student: Blazquez Fernandez Samuel

Obtained qualification: Sobresaliente cum Laude for unanimidad

Date of reading: 29/10/2024

European doctorate: Yes **Date of recognition:** 29/10/2024

Date of award: 29/10/2024



- 2** **Project title:** Estudio termodinámico y científico de los cambios de fase por dinámica molecular
Type of project: Doctoral thesis
Co-director of thesis: Sanz E.; Noya E.G.; Vega C
Entity: Universidad Complutense de Madrid **Type of entity:** University
Student: Pulido Lamas Cintia
Obtained qualification: Sobresaliente cum Laude por Unanimidad
Date of reading: 15/02/2024
European doctorate: Yes **Date of recognition:** 15/02/2024
- 3** **Project title:** Cinética de la cristalización
Type of project: Doctoral thesis
Entity: Universidad Complutense de Madrid **Type of entity:** University
Student: Pablo Montero de Hijes
Obtained qualification: Sobresaliente cum Laude por Unanimidad
Date of reading: 17/12/2021
- 4** **Project title:** Estudio por simulación de transiciones de fase iniciadas por nucleación
Type of project: Doctoral thesis
Co-director of thesis: Chantal Valeriani; Eduardo Sanz Garcia
Entity: Universidad Complutense de Madrid **Type of entity:** University
Student: Pablo Rosales Pelaez
Obtained qualification: Sobresaliente cum Laude por Unanimidad
Date of reading: 30/11/2020
- 5** **Project title:** Nucleación de sólidos cristalinos por simulación
Type of project: Doctoral thesis
Co-director of thesis: Eduardo Sanz Garcia
Entity: Universidad Complutense de Madrid **Type of entity:** University
City of entity: Madrid, Community of Madrid, Spain
Student: Jorge Reñe Espinosa
Obtained qualification: Apto cum Laude por unanimidad
Date of reading: 23/02/2018
European doctorate: Yes **Date of recognition:** 23/02/2018
- 6** **Project title:** Simulación del equilibrio de fases del agua: cristales plásticos, constantes dieléctricas y disoluciones
Type of project: Doctoral thesis
Entity: Universidad Complutense de Madrid **Type of entity:** University
City of entity: Madrid, Community of Madrid, Spain
Student: JUAN LUIS ARAGONES GOMEZ
Obtained qualification: Apto, Premio Extraordinario de Doctorado
Date of reading: 05/10/2012
- 7** **Project title:** Simulación del equilibrio de fases de agua: hielos e hidratos
Type of project: Doctoral thesis
Entity: Universidad Complutense de Madrid **Type of entity:** University
City of entity: Madrid, Community of Madrid, Spain
Student: MARIA MARTIN CONDE
Obtained qualification: Apto, Premio Extraordinario de Doctorado
Date of reading: 06/10/2011

- 8** **Project title:** Equilibrio termodinámico de sólidos mediante simulación molecular.
Type of project: Doctoral thesis
Entity: Universidad Complutense de Madrid **Type of entity:** University
City of entity: Madrid, Community of Madrid, Spain
Student: EUDARDO SANTIAGO SANZ GARCIA
Obtained qualification: Sobresaliente Cum Laude, Premio Extraordinario de Doctorado
Date of reading: 13/01/2006
- 9** **Project title:** Termodinámica Estadística de moléculas flexibles : teoría y simulación
Type of project: Doctoral thesis
Entity: Universidad Complutense de Madrid **Type of entity:** University
City of entity: Madrid, Community of Madrid, Spain
Student: LUIS GONZALEZ MAC-DOWELL
Obtained qualification: Sobresaliente cum laude
Date of reading: 20/05/2000

Scientific and technological experience

Scientific or technological activities

R&D projects funded through competitive calls of public or private entities

- 1** **Name of the project:** PID2022-136919NB-C31 Aspectos fundamentales de la simulación molecular de la cinética y la termodinámica de transiciones de fase de sistemas de interés tecnológico y biológico
City of entity: Spain
Name principal investigator (PI, Co-PI....): Eduardo Sanz; Carlos Vega
Nº of researchers: 3
Start-End date: 01/09/2023 - 01/09/2026
Total amount: 60.000 €
- 2** **Name of the project:** PID2019-105898GB-C21 ASPECTOS FUNDAMENTALES DE LA SIMULACION DE LA NUCLEACION EN MATERIA CONDENSADA
Name principal investigator (PI, Co-PI....): Eduardo Sanz Garcia; Carlos Vega de las Heras
Nº of researchers: 3
Start-End date: 01/06/2020 - 01/06/2023
Total amount: 85.000 €
- 3** **Name of the project:** FIS2016-78117-P MODELADO DE LA CRISTALIZACION EN DISOLUCION
Name principal investigator (PI, Co-PI....): Carlos Vega De las Heras; Eduardo Sanz García
Nº of researchers: 4
Start-End date: 01/01/2017 - 01/01/2020
Total amount: 80.000 €
- 4** **Name of the project:** FIS2013-43209-P Termodinámica y Cinética de la Transición Líquido-Sólido mediante simulación molecular: agua, disoluciones y otros sistemas
Entity where project took place: Universidad **Type of entity:** University
Complutense de Madrid
City of entity: Madrid,



Name principal investigator (PI, Co-PI....): Carlos Vega de las Heras; Eduardo Sanz García

Nº of researchers: 5

Start-End date: 01/01/2014 - 31/03/2018

Total amount: 87.000 €

5 Name of the project: FIS2010-16159 SIMULACIONES CLASICAS Y CUANTICAS DEL AGUA Y DE SU EQUILIBRIO DE FASES

Type of project: Research and development, including transfer

Geographical area: National

Name principal investigator (PI, Co-PI....): CARLOS VEGA DE LAS HERAS

Nº of researchers: 4

Funding entity or bodies:

MINISTERIO DE CIENCIA E INNOVACIÓN

Start-End date: 31/12/2010 - 31/12/2013

Duration: 3 years - 1 day

Total amount: 85.000 €

Dedication regime: Full time

6 Name of the project: MODELICO, P2009/ESP-1691 MODELIZACION Y SIMULACION DE SISTEMAS COMPLEJOS. MODELICO

Type of project: Research and development, including transfer

Geographical area: Regional

Name principal investigator (PI, Co-PI....): CARLOS VEGA DE LAS HERAS

Nº of researchers: 5

Funding entity or bodies:

Comunidad de Madrid

Type of entity: Comunidad de Madrid

City funding entity: Madrid, Community of Madrid, Spain

Start-End date: 01/01/2010 - 31/12/2013

Duration: 4 years - 1 day

Total amount: 90.000 €

Dedication regime: Full time

7 Name of the project: GR58/08 Simulación por ordenador y modelado mecanoestadístico de líquidos y sólidos

Type of project: Research and development, including transfer

Entity where project took place: Universidad Complutense de Madrid

Type of entity: University

City of entity: Community of Madrid, Spain

Name principal investigator (PI, Co-PI....): JOSE LUIS FERNANDEZ ABASCAL; Carlos Vega de las Heras

Nº of researchers: 7

Funding entity or bodies:

Universidad Complutense de Madrid

Type of entity: University

City funding entity: Madrid, Community of Madrid, Spain

Start-End date: 01/01/2009 - 31/12/2010

Duration: 2 years - 4 days

Total amount: 9.000 €

Dedication regime: Full time

8 Name of the project: FIS2007-66079-C02-01 Simulación por ordenador del equilibrio de las fases del agua

Type of project: Research and development, including transfer

Name principal investigator (PI, Co-PI....): CARLOS VEGA DE LAS HERAS

Nº of researchers: 7

**Funding entity or bodies:**

MINISTERIO DE CIENCIA E INNOVACIÓN

Start-End date: 01/10/2007 - 30/09/2010**Duration:** 3 years**Total amount:** 60.000 €**Dedication regime:** Full time

- 9** **Name of the project:** Mossnoho, S-0505/ESP/0299 Modelización y simulación de sistemas no homogéneos en materia condensada

Type of project: Research and development, including transfer**Name principal investigator (PI, Co-PI....):** CARLOS VEGA DE LAS HERAS**Nº of researchers:** 4**Funding entity or bodies:**

Comunidad de Madrid

Type of entity: Comunidad de Madrid**City funding entity:** Madrid, Community of Madrid, Spain**Start-End date:** 01/01/2006 - 31/12/2009**Duration:** 4 years**Total amount:** 138.753 €**Dedication regime:** Full time

- 10** **Name of the project:** MTKD-CT-2004-509249 THEORY AND COMPUTER SIMULATION OF INTERFACIAL PHENOMENA, Marie Curie Host Fellowships for the transfer or knowledge
- Type of project:** Research and development, including transfer

Geographical area: European Union**Name principal investigator (PI, Co-PI....):** CARLOS VEGA DE LAS HERAS**Nº of researchers:** 2**Funding entity or bodies:**

Unión Europea

Start-End date: 01/03/2005 - 01/03/2008**Duration:** 3 years - 1 day**Total amount:** 200.000 €**Dedication regime:** Full time

- 11** **Name of the project:** FIS2004-06227-C02-02 Modelización molecular del equilibrio de fases de sistemas de interés tecnológico y/o biológico

Type of project: Research and development, including transfer**Name principal investigator (PI, Co-PI....):** CARLOS VEGA DE LAS HERAS**Nº of researchers:** 5**Funding entity or bodies:**

MINISTERIO DE CIENCIA E INNOVACIÓN

Start-End date: 13/12/2004 - 12/12/2007**Duration:** 3 years - 4 days**Total amount:** 41.833 €**Dedication regime:** Full time

- 12** **Name of the project:** BFM2001-1420-C02-01 MECANICA ESTADISTICA DE SISTEMAS COMPLEJOS: MOLECULAS FLEXIBLES Y MESOFASE

Type of project: Research and development, including transfer**Name principal investigator (PI, Co-PI....):** CARLOS VEGA DE LAS HERAS**Nº of researchers:** 4**Funding entity or bodies:**

MINISTERIO DE CIENCIA E INNOVACIÓN

Start-End date: 01/01/2002 - 27/12/2004**Duration:** 2 years - 7 months - 10 days



Total amount: 18.000 €

Dedication regime: Full time

13 Name of the project: PB97-0329 TEORIA Y SIMULACION DE TRANSICIONES DE FASE EN SISTEMAS COMPLEJOS: HIDROCARBUROS Y CRISTALES LIQUIDOS

Type of project: Research and development, including transfer

Name principal investigator (PI, Co-PI....): CARLOS VEGA DE LAS HERAS

Nº of researchers: 6

Funding entity or bodies:

MINISTERIO DE CIENCIA E INNOVACIÓN

Start-End date: 01/11/1998 - 01/11/2001

Duration: 3 years - 1 day

Total amount: 18.000 €

Dedication regime: Full time

14 Name of the project: PB94-0285 ESTUDIO TEORICO Y DE SIMULACION DE LIQUIDOS MOLECULARES COMPLEJOS CON POSIBLES APLICACIONES EN DIFERENTES CAMPOS CIENTIFICOS E INDUSTRIALES.

Type of project: Research and development, including transfer

Degree of contribution: Researcher

Name principal investigator (PI, Co-PI....): SANTIAGO LAGO ARANDA

Nº of researchers: 5

Funding entity or bodies:

MINISTERIO DE CIENCIA E INNOVACIÓN

Start-End date: 15/06/1995 - 15/06/1998

Duration: 3 years

Total amount: 30.471 €

Dedication regime: Full time

15 Name of the project: PB91-0364 INFLUENCIA DE LA FLEXIBILIDAD MOLECULAR Y LOS MOMENTOSMULTIPOLARES EN LAS PROPIEDADES TERMODINAMICAS DE LIQUIDOS

Type of project: Research and development, including transfer

Geographical area: National

Degree of contribution: Researcher

Name principal investigator (PI, Co-PI....): SANTIAGO LAGO ARANDA

Nº of researchers: 2

Funding entity or bodies:

MINISTERIO DE CIENCIA E INNOVACIÓN

Start-End date: 01/01/1993 - 23/12/1995

Duration: 2 years - 11 months - 26 days

Total amount: 25.000 €

Dedication regime: Full time

R&D non-competitive contracts, agreements or projects with public or private entities

1 Name of the project: Marie Curie Post-doctoral fellowship (Contrato Valentino Bianco)

Funding entity or bodies:

Union Europea

Start date: 01/09/2018

Duration: 2 years

Total amount: 130.000 €

**2 Name of the project:** Juan de la Cierva fellowship (Contrato Chantal Valeriani)**Type of project:** Research and development, including transfer**Degree of contribution:** Researcher**Name principal investigator (PI, Co-PI....):** CARLOS VEGA DE LAS HERAS**Nº of researchers:** 2**Funding entity or bodies:**

MINISTERIO DE CIENCIA E INNOVACIÓN

Start date: 01/05/2011**Duration:** 3 years - 1 day**Total amount:** 60.000 €**3 Name of the project:** Juan de la Cierva , fellowship (Contrato Eva González Noya)**Type of project:** Research and development, including transfer**Degree of contribution:** Researcher**Name principal investigator (PI, Co-PI....):** CARLOS VEGA DE LAS HERAS**Nº of researchers:** 2**Funding entity or bodies:**

MINISTERIO DE CIENCIA E INNOVACIÓN

Start date: 01/12/2006**Duration:** 3 years - 10 months - 4 days**Total amount:** 60.000 €**4 Name of the project:** Marie Curie Post-Doctoral Fellowship (Contrato Carl McBride)**Funding entity or bodies:**

Union Europea

Start date: 01/08/2000**Duration:** 2 years**Total amount:** 110.000 €

Scientific and technological activities

Scientific production

H index: 63**Date of application:** 20/02/2025**Source of H-Index:** WOS

Publications, scientific and technical documents

- 1** Samuel Blazquez; Ian C Bourgh; Carlos Vega. Madrid-2019 force field: An extension to divalent cations Sr^{2+} and Ba^{2+} . Journal of Chemical Physics. 160, pp. 046101. AIP, 25/01/2024.

Type of production: Scientific paper**Format:** Journal**Corresponding author:** Yes**Relevant publication:** Yes

- 2** Diego G Salgado; Carlos Vega. A new interaction potential for Cl^- , Li^+ , Na^+ , and Ca^{2+} in methanol solutions using the scaled charges concept. Journal of Chemical Physics. 162, pp. 074502. 19/02/2025.

Type of production: Scientific paper**Total no. authors:** 2**Corresponding author:** No



- 3** Lucia F. Sedano; Carlos Vega; Eva G. Noya; Eduardo Sanz. TIP4P2005Ice: Simulating water with two molecular states. Journal of Chemical Physics. 162, pp. 014502. 07/01/2025.
Type of production: Scientific paper
Total no. authors: 4
Corresponding author: No
- 4** Samuel Blazquez; Lucia F Sedano; Carlos Vega. On the compatibility of the Madrid-2019 force field for electrolytes with the TIP4P/Ice water model. Journal of Chemical Physics. 161, pp. 224502. 14/12/2024.
Type of production: Scientific paper
Total no. authors: 3
Format: Journal
Corresponding author: Yes
- 5** Ignacio Sanchez Burgos; Pablo M de Hijes; Eduardo Sanz; Carlos Vega; Jorge R Espinosa. Predictions of the interfacial free energy along the coexistence line from single-state calculations. Journal of Chemical Physics. 161, pp. 204701. 20/11/2024.
Type of production: Scientific paper
Total no. authors: 5
Format: Journal
Corresponding author: No
- 6** Cintia P Lamas; Carlos Vega; Paola Gallo. Impact of sulfate salts on water structure: insights from molecular dynamics. Molecular Physics. 122, pp. e2406260. 16/11/2024.
Type of production: Scientific paper
Total no. authors: 3
Format: Journal
Corresponding author: No
- 7** Marjolein de Jager; Carlos Vega; Pablo M de Hijes; Frank Smullenburg; Laura Filion. Statistical mechanics of crystal nuclei of hard spheres. Journal of Chemical Physics. 161, pp. 184501. 06/11/2024.
Type of production: Scientific paper
Total no. authors: 5
Corresponding author: No
- 8** Lucia F. Sedano; Carlos Vega; Eva G. Noya. Isothermal compressibility and water self-diffusion coefficient in supercooled salt aqueous solutions using the Madrid-2019 model. Molecular Physics. 122 - 21-22, pp. e2418311. 22/10/2024.
Type of production: Scientific paper
Total no. authors: 3
Format: Journal
Corresponding author: No
- 9** Marcos de Lucas; Samuel Blazquez; Jacobo Troncoso; Carlos Vega; Francisco Gamez. Dressing a Nonpolarizable Force Field for OH⁻ in TIP4P/2005 Aqueous Solutions with Corrected Hirshfeld Charges. The Journal of Physical Chemistry Letters. 15, pp. 9411. 09/09/2024.
Type of production: Scientific paper
Total no. authors: 5
Corresponding author: No
- 10** Lucia F Sedano; Samuel Blazquez; Carlos Vega. Accuracy limit of non-polarizable four-point water models: TIP4P/2005 vs OPC. Should water models reproduce the experimental dielectric constant?. Journal of Chemical Physics. 161, pp. 044505. 28/07/2024.
Type of production: Scientific paper
Total no. authors: 3
- 11** Samuel Blazquez; Marcos de Lucas; Carlos Vega; Jacobo Troncoso; Francisco Gamez. The temperature of maximum in density of aqueous solutions of nitrate and ammonium salts: Testing the Madrid-2019 force field. Journal of Chemical Physics. 161, pp. 046103. 28/07/2024.
Type of production: Scientific paper
Total no. authors: 5
Format: Journal



- 12** Willem Gispen; Jorge R Espinosa; Eduardo Sanz; Carlos Vega; Marjolein Dijkstra. Variational umbrella seeding for calculating nucleation barriers. *Journal of Chemical Physics*. 160, pp. 174501. 15/05/2024.
Type of production: Scientific paper **Format:** Journal
Total no. authors: 5
- 13** Samuel Blazquez; Jesus Algaba; Jose M Miguez; Carlos Vega; Felipe J Blas; Maria M Conde. Three-phase equilibria of hydrates from computer simulation. I. Finite-size effects in the methane hydrate. *Journal of Chemical Physics*. 160, pp. 164721. 28/04/2024.
Type of production: Scientific paper **Format:** Journal
Total no. authors: 6 **Corresponding author:** No
- 14** Parsa Habibi; H Mert Polat Polat; Samuel Blazquez; Carlos Vega; Poulumi Dey; Thijs JH Vlugt; Othonas A Moulτος. Accurate Free Energies of Aqueous Electrolyte Solutions from Molecular Simulations with Non-polarizable Force Fields. *The Journal of Physical Chemistry Letters*. 15, pp. 4477. 18/04/2024.
Type of production: Scientific paper **Corresponding author:** No
Total no. authors: 7
- 15** Andres R Tejedor; Ignacio Sanchez Burgos; Eduardo Sanz; Carlos Vega; Felipe J Blas; Ruslan Davidchack; Nicodemo di Pasquale; Jorge Ramirez; Jorge R Espinosa. Mold: a LAMMPS package to compute interfacial free energies and nucleation rates. *Journal of Open Source Software*. 9, pp. 6083. 26/03/2024.
Type of production: Scientific paper **Format:** Journal
Total no. authors: 9 **Corresponding author:** No
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Type of production: Scientific paper **Format:** Journal
Total no. authors: 3 **Corresponding author:** Yes
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Type of production: Scientific paper **Format:** Journal
Corresponding author: No
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Type of production: Scientific paper
Corresponding author: No
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Type of production: Scientific paper
Corresponding author: Yes
Source of citations: WOS **Citations:** 3
- 20** J.R. Espinosa; J.L.F. Abascal; L.F. Sedano; E. Sanz; C. Vega. On the possible locus of the liquid-liquid critical point in real water from studies of supercooled water using the TIP4P/Ice model. *Journal of Chemical Physics*. 158, pp. 204505. 25/05/2023.
Type of production: Scientific paper
Corresponding author: Yes

- 21** J. Algaba; I.M. Zeron; J.M. Miguez; J Grabowska; S Blazquez; E Sanz; C Vega; F. J. Blas. Solubility of carbon dioxide in water: Some useful results for hydrate nucleation. Journal of Chemical Physics. 158, pp. 184703. 09/05/2023.
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Type of production: Scientific paper
Corresponding author: No
Source of citations: SCOPUS **Citations:** 5
- 23** C.P. Lamas; C. Vega; E.G. Noya; E. Sanz. The water cavitation line as predicted by the TIP4P/2005 model. Journal of Chemical Physics. 158, pp. 124504. 24/03/2023.
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Corresponding author: No
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Corresponding author: No
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Corresponding author: No
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Corresponding author: Yes

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Type of production: Scientific paper

Format: Journal

Corresponding author: Yes

Source of citations: SCOPUS

Citations: 13

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Format: Journal

Corresponding author: Yes

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Type of production: Scientific paper

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Type of production: Scientific paper

Format: Journal

Corresponding author: Yes

Source of citations: SCOPUS

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Type of production: Scientific paper

Format: Journal

Corresponding author: Yes

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Corresponding author: Yes
Source of citations: WOS **Citations:** 23
- 42** I Sanchez-Burgos; P Montero de Hijes; P Rosales-Pelaez; C Vega; E Sanz. Equivalence between condensation and boiling in a Lennard-Jones fluid. *Physical Review E*. 102, pp. 062609. 28/12/2020.
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Corresponding author: Yes
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Source of citations: WOS **Citations:** 28
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Type of production: Scientific paper**Format:** Journal

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Type of production: Scientific paper **Format:** Journal
Position of signature: 5
Total no. authors: 6
Impact source: ISI
Impact index in year of publication: 9,353
Source of citations: WOS **Citations:** 9
Relevant results: 9 citas
Relevant publication: No
- 63** A.L. Benavides; M.A. Portillo; V.C. Chamorro; J.R. Espinosa; J.L.F. Abascal; C. Vega. A potential model for sodium chloride solutions based on the TIP4P/2005 water model. *Journal of Chemical Physics*. 147, pp. 104501. 14/09/2017. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 6
Total no. authors: 6
Impact source: ISI
Impact index in year of publication: 2,965
- 64** R. Lustig; C. Vega; J. Vrabec. Special Issue of Molecular Physics in Honour of Professor Johann Fischer. *Molecular Physics*. 115, pp. 1015. 15/06/2017. ISSN 0026-8976
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Type of production: Scientific paper **Format:** Journal
Impact source: ISI
Impact index in year of publication: 1,87
Source of citations: WOS **Citations:** 1
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Impact source: ISI
Impact index in year of publication: 3,588
- 67** J.R. Espinosa; C. Navarro; E. Sanz; C. Valeriani; C. Vega. On the time required to freeze water. *Journal of Chemical Physics*. 145, pp. 211922. 21/12/2016. ISSN 0021-9606
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Position of signature: 5
Total no. authors: 5



Impact source: ISI

Impact index in year of publication: 2,965

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Citations: 5

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Format: Journal

Impact source: ISI

Impact index in year of publication: 2,965

Source of citations: WOS

Citations: 8

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Type of production: Scientific paper

Position of signature: 6

Total no. authors: 7

Impact source: ISI

Impact index in year of publication: 8,462

Source of citations: WOS

Citations: 5

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Format: Journal

Impact source: ISI

Impact index in year of publication: 2,965

Source of citations: WOS

Citations: 4

- 71** P. Gallo; K. Arnann-Winkel; CA Angell; MA Anisimov; F. Caupin; C. Chakravarty; E. Lascaris; T. Loerting; AZ Panagiotopoulos; J Russo; JA Sellberg; HE Stanley; H. Tanaka; C. Vega; LM Xu; LGM Pettersson. Water a Tale of Two Liquids. *Chemical Reviews*. 116, pp. 7463 - 7500. 13/07/2016. ISSN 0009-2665

Type of production: Scientific paper

Format: Journal

Position of signature: 14

Total no. authors: 16

Impact source: ISI

Impact index in year of publication: 47,93

Source of citations: WOS

Citations: 54

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Type of production: Scientific paper

Format: Journal

Position of signature: 2

Total no. authors: 3

Impact source: ISI

Impact index in year of publication: 4,536

Source of citations: WOS

Citations: 14

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Type of production: Scientific paper

Format: Journal

Position of signature: 3

Total no. authors: 3

Impact source: ISI

Impact index in year of publication: 2,965

Source of citations: WOS

Citations: 15

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Type of production: Scientific paper

Format: Journal

Position of signature: 2

Total no. authors: 4

Impact source: ISI

Impact index in year of publication: 2,965

Source of citations: WOS

Citations: 28

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Type of production: Scientific paper

Format: Journal

Impact source: ISI

Impact index in year of publication: 2,894

Source of citations: WOS

Citations: 20

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Format: Journal

Impact source: ISI

Impact index in year of publication: 2,894

Source of citations: WOS

Citations: 15

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Type of production: Scientific paper

Format: Journal

Source of citations: WOS

Citations: 5

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Format: Journal



Impact source: ISI

Impact index in year of publication: 1,837

Source of citations: WOS

Citations: 20

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Format: Journal

Impact source: ISI

Impact index in year of publication: 1,837

Source of citations: WOS

Citations: 7

- 80** J.M. Miguez; M.M. Conde; J.P. Torre; F.J. Blas; M. Piñeiro; C Vega. Molecular dynamics simulation of CO₂ hydrates: Prediction of three phase coexistence line. Journal of Chemical Physics. 142, pp. 124505. 28/03/2015. ISSN 0021-9606

Type of production: Scientific paper

Impact source: ISI

Impact index in year of publication: 2,894

Source of citations: WOS

Citations: 20

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Format: Journal

Impact source: ISI

Impact index in year of publication: 4,493

Source of citations: WOS

Citations: 5

- 82** Jorge Reñe; Eduardo Sanz; Chantal Valeriani; Carlos Vega. Homogeneous ice nucleation evaluated for several water models. Journal of Chemical Physics. 141, pp. 18C529 - 18C529. American Institute of Physics, 14/11/2014. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Impact source: ISI

Impact index in year of publication: 2,952

Source of citations: WOS

Citations: 38

- 83** Jorge Reñe Espinosa; Carlos Vega; Eduardo Sanz. The mold integration method for the calculation of the crystal-fluid interfacial free energy from simulations. Journal of Chemical Physics. 141, pp. 044715 - 044715. American Institute of Physics, 07/10/2014. ISSN 0021-9606

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Format: Journal

Impact source: ISI

Impact index in year of publication: 2,952

Source of citations: WOS

Citations: 17

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Impact source: ISI
Impact index in year of publication: 3,302
Source of citations: WOS

Citations: 19

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Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 3,122

Format: Journal

Source of citations: WOS

Citations: 20

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Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 3.122

Source of citations: WOS

Citations: 26

- 87** Eduardo Sanz; Carlos Vega de las Heras; Jorge Reñe Espinosa; Ruth Caballero Bernal; Jose Luis Fernandez Abascal; Chantal Valeriani. Homogeneous Ice Nucleation at Moderate Supercooling from Molecular Simulation. Journal of the American Chemical Society. 135, pp. 15008 - 15017. 09/10/2013. ISSN 0002-7863

Type of production: Scientific paper
Position of signature: 2
Total no. authors: 6
Impact source: ISI
Impact index in year of publication: 11,444

Source of citations: WOS

Citations: 91

- 88** Guadalupe Jimenez Serratos; Alejandro Gil Villegas; Carlos Vega de las Heras; Felipe Jimenez Blas. Monte Carlo simulation of flexible trimers: From square well chains to amphiphilic primitive models. Journal of Chemical Physics. 139, pp. 114901. 21/09/2013. ISSN 0021-9606

Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 3.122

Source of citations: WOS

Citations: 4

- 89** Jonathan B. Boreyko; Bernadeta R. Srijanto; Trung Dac Nguyen; Carlos Vega de las Heras; Miguel Fuentes Cabrera; C. Patrick Collier. Dynamic Defrosting on Nanostructured Superhydrophobic Surfaces. Langmuir. 29, pp. 9516 - 9524. 30/07/2013. ISSN 0743-7463

Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 4.384

Source of citations: WOS

Citations: 56



- 90** Juan Luis Aragonés Gómez; Eva González Noya; Chantal Valeriani; Carlos Vega de las Heras. Free energy calculations for molecular solids using GROMACS. *Journal of Chemical Physics*. 139, pp. 034104. 21/07/2013. ISSN 0021-9606
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Impact source: ISI
Impact index in year of publication: 3.122
Source of citations: WOS
Citations: 14
- 91** CARL MCBRIDE; EVA GONZALEZ NOYA; CARLOS VEGA DE LAS HERAS. A computer program to evaluate the NVM propagator for rigid asymmetric tops for use in path integral simulations of rigid bodies. *Computer Physics Communications*. 184, pp. 885 - 890. (Holland): 01/03/2013. ISSN 0010-4655
Type of production: Scientific paper
Format: Journal
Impact source: ISI
Impact index in year of publication: 2,407
Source of citations: WOS
Citations: 6
- 92** German Pérez Sánchez; Diego González Salgado; Manuel Martínez Piñeiro; Carlos Vega de las Heras. Fluid-solid equilibrium of carbon dioxide as obtained from computer simulations of several popular potential models: The role of the quadrupole. *Journal of Chemical Physics*. 138, pp. 084506. 28/02/2013. ISSN 0021-9606
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 3.122
Source of citations: WOS
Citations: 12
- 93** MARIA MARTIN CONDE; CARLOS VEGA DE LAS HERAS. A simple correlation to locate the three phase coexistence line in methane hydrate simulations. *Journal of Chemical Physics*. 138, pp. 056101 - 056101. (United States of America): 07/02/2013. ISSN 0021-9606
Type of production: Scientific paper
Format: Journal
Impact source: ISI
Impact index in year of publication: 3,122
Source of citations: WOS
Citations: 18
- 94** Guadalupe Jiménez-Serratos; CARLOS VEGA DE LAS HERAS; Alejandro Gil-Villegas. Evaluation of the pressure tensor and surface tension for molecular fluids with discontinuous potentials using the volume perturbation method, volumen 137, 204104. *Journal of Chemical Physics*. 137, pp. 204104 - 204104. (United States of America): 28/11/2012. ISSN 0021-9606
Type of production: Scientific paper
Format: Journal
Impact source: ISI
Impact index in year of publication: 3,164
Source of citations: WOS
Citations: 6
- 95** CARLOS VEGA DE LAS HERAS; Stefan Sokolowski. Orest Pizio: scientist and friend Foreword. *Condensed Matter Physics*. 15, pp. 20101 - 20101. (Ukraine): 01/11/2012. ISSN 1607-324X
Type of production: Scientific paper
Format: Journal
Position of signature: 1



- 96** JUAN LUIS ARAGONES GOMEZ; C. Valeriani; CARLOS VEGA DE LAS HERAS. Free energy calculations for atomic solids through the Einstein crystal/molecule methodology using GROMACS and LAMMPS. Journal of Chemical Physics. 137, pp. 146101 - 146101. (United States of America): 14/10/2012. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Impact source: ISI

Impact index in year of publication: 3,164

Source of citations: WOS

Citations: 17

- 97** Aleks Reinhardt; J. P. K. Doye; EVA GONZALEZ NOYA; CARLOS VEGA DE LAS HERAS. Local order parameters for use in driving homogeneous ice nucleation with all-atom models of water, volumen 137, 194504, 0 citas. Journal of Chemical Physics. 137, pp. 194504 - 194504. (United States of America): 21/09/2012. ISSN 0021-9606

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Format: Journal

Impact source: ISI

Impact index in year of publication: 3,164

Source of citations: WOS

Citations: 36

- 98** CARL MCBRIDE; JUAN LUIS ARAGONES GOMEZ; EVA GONZALEZ NOYA; CARLOS VEGA DE LAS HERAS. A study of the influence of isotopic substitution on the melting point and temperature of maximum density of water by means of path integral simulations of rigid models. Physical Chemistry Chemical Physics. 14, pp. 15199 - 15205. (United Kingdom): 15/09/2012. ISSN 1463-9076

Type of production: Scientific paper

Format: Journal

Impact source: ISI

Impact index in year of publication: 3,829

Source of citations: WOS

Citations: 7

- 99** JUAN LUIS ARAGONES GOMEZ; EDUARDO SANZ GARCIA; C. Valeriani; CARLOS VEGA DE LAS HERAS. Calculation of the melting point of alkali halides by means of computer simulations. Journal of Chemical Physics. 137, pp. 104507 - 104507. (United States of America): 14/09/2012. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Impact source: ISI

Impact index in year of publication: 3,164

Source of citations: WOS

Citations: 15

- 100** JUAN LUIS ARAGONES GOMEZ; EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. Solubility of NaCl in water by molecular simulation revisited. Journal of Chemical Physics. 136, pp. 244508 - 244508. (United States of America): 28/06/2012. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Impact source: ISI

Impact index in year of publication: 3,164

Source of citations: WOS

Citations: 61

- 101** CARL MCBRIDE; EVA GONZALEZ NOYA; JUAN LUIS ARAGONES GOMEZ; MARIA MARTIN CONDE; CARLOS VEGA DE LAS HERAS. The phase diagram of water from quantum simulations. Physical Chemistry Chemical Physics. 14, pp. 10140 - 10146. (United Kingdom): 01/05/2012. ISSN 1463-9076

Type of production: Scientific paper

Format: Journal

Impact source: ISI



Impact index in year of publication: 3,829

Source of citations: WOS

Citations: 20

- 102** JOSE LUIS FERNANDEZ ABASCAL; CARLOS VEGA DE LAS HERAS. Physics and chemistry of water and ice. Physical Chemistry Chemical Physics. 13, pp. 19660 - 19662. (United Kingdom): 30/11/2011. ISSN 1463-9076

Type of production: Scientific paper

Format: Journal

Impact source: ISI

Impact index in year of publication: 3,6

Source of citations: WOS

Citations: 5

- 103** JOSE LUIS FERNANDEZ ABASCAL; CARLOS VEGA DE LAS HERAS. Simulating water with rigid non-polarizable models: a general perspective. Physical Chemistry Chemical Physics. 13, pp. 19663 - 19688. (United Kingdom): 01/11/2011. ISSN 1463-9076

Type of production: Scientific paper

Format: Journal

Position of signature: 2

Total no. authors: 2

Source of citations: WOS

Citations: 211

- 104** Juan Luis Aragonés; Luis G. MacDowell; J. I. Siepmann; Carlos Vega. Phase Diagram of Water under an Applied Electric Field. Physical Review Letters. 107, pp. 155702. 12/10/2011.

Type of production: Scientific paper

Format: Journal

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Citations: 20

- 105** ANA DOPAZO PAZ; PEDRO GOMEZ ALVAREZ; DIEGO GONZALEZ SALGADO; J M MINGUEZ; CARLOS VEGA DE LAS HERAS. Solid-solid and solid-fluid equilibria of the most popular models of methanol obtained by computer simulation. Journal of Physical Chemistry B Materials. 115, pp. 3522 - 3532. (United States of America): 01/07/2011. ISSN 1089-5647

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Format: Journal

Impact source: ISI

Impact index in year of publication: 3,8

Source of citations: WOS

Citations: 5

- 106** JUAN LUIS ARAGONES GOMEZ; LUIS GONZALEZ MAC-DOWELL; CARLOS VEGA DE LAS HERAS. The dielectric constant of ice and water: A lesson about the water interactions, volumen 115, Impacto 3,2, 13 citas. The journal of physical chemistry. A, Molecules, spectroscopy, kinetics, environment & general theory. 115, pp. 5745 - 5755. (United States of America): 01/06/2011. ISSN 1089-5639

Type of production: Scientific paper

Format: Journal

Source of citations: WOS

Citations: 33

- 107** JOSE LUIS FERNANDEZ ABASCAL; CARLOS VEGA DE LAS HERAS. Note: Equation of state and compressibility of supercooled water: Simulations and experiment. Journal of Chemical Physics. 134, pp. 186101 - 186101. (United States of America): 01/05/2011. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Source of citations: WOS

Citations: 28

- 108** JOSE EMILIO FERNANDEZ RUBIO; RAMON GONZALEZ RUBIO; LAURA JIMENEZ BONALES; FRANCISCO ORTEGA GOMEZ; HERNAN ALEJANDRO RITACCO; CARLOS VEGA DE LAS HERAS. Freezing transition and interaction potential in monolayers of microparticles at fluid interfaces. *Langmuir : the ACS journal of surfaces and colloids*. 27, pp. 3391 - 3400. (United States of America): 01/04/2011. ISSN 0743-7463
Type of production: Scientific paper **Format:** Journal
Impact source: ISI
Impact index in year of publication: 4,2
Source of citations: WOS **Citations:** 20
- 109** EVA GONZALEZ NOYA; CARL MCBRIDE; CARLOS VEGA DE LAS HERAS. A quantum propagator for path-integral simulations of rigid molecules. *Journal of Chemical Physics*. 134, pp. 054117 - 054117. (United States of America): 01/03/2011. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Source of citations: WOS **Citations:** 14
- 110** CARL MCBRIDE; MARIA MARTIN CONDE; EVA GONZALEZ NOYA; CARLOS VEGA DE LAS HERAS. Path integral Monte Carlo simulations for rigid rotors and their application to water. *Molecular Physics*. 109, pp. 149 - 168. (United Kingdom): 15/01/2011. ISSN 0026-8976
Type of production: Scientific paper **Format:** Journal
Impact source: ISI
Impact index in year of publication: 1.7
Source of citations: WOS **Citations:** 16
- 111** JOSE LUIS FERNANDEZ ABASCAL; CARLOS VEGA DE LAS HERAS. Widom line and the liquid-liquid critical point for the TIP4P/2005 water model. *Journal of Chemical Physics*. 133, pp. 234502 - 234502. (United States of America): 15/12/2010. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Total no. authors: 2
Impact source: ISI
Impact index in year of publication: 3,33
Source of citations: WOS **Citations:** 103
- 112** Briesta S. Gonzalez; Eva G. Noya; LUIS M. SESE; CARLOS VEGA DE LAS HERAS. Nuclear Quantum Effects in Water Clusters: The Role of the Molecular Flexibility. *Journal of Physical Chemistry B*. 114, pp. 2484 - 2492. (United States of America): 08/10/2010. ISSN 1520-6106
Type of production: Scientific paper **Format:** Journal
Position of signature: 3
Source of citations: WOS **Citations:** 21
- 113** CARLOS VEGA DE LAS HERAS; LUIS GONZALEZ MAC-DOWELL. Dielectric Constant of Ice Ih and Ice V: A Computer Simulation Study. *Journal of Physical Chemistry B Materials*. 114, pp. 6089 - 6098. (United States of America): 01/10/2010. ISSN 1089-5647
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Source of citations: WOS **Citations:** 20

- 114** MARIA MARTIN CONDE; CARLOS VEGA DE LAS HERAS. Determining the three-phase coexistence line in methane hydrates using computer simulations. Journal of Chemical Physics. 133, pp. 064507 - 064507. (United States of America): 15/08/2010. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Total no. authors: 2
Source of citations: WOS **Citations:** 57
- 115** Maria M. Conde; CARL MCBRIDE; Eva G. Noya; RAFAEL RAMIREZ; LUIS M. SESE; CARLOS VEGA DE LAS HERAS. Can gas hydrate structures be described using classical simulations?. Journal of Chemical Physics. 132, pp. 114503 - 114503. (United States of America): 01/08/2010. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Source of citations: WOS **Citations:** 17
- 116** J PK DOYE; EVA GONZALEZ NOYA; AA LOUIS; CARLOS VEGA DE LAS HERAS. The stability of a crystal with diamond structure for patchy particles with tetrahedral symmetry. Journal of Chemical Physics. 132, pp. 234511 - 234511. (United States of America): 01/06/2010. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Source of citations: WOS **Citations:** 49
- 117** DIEGO GONZALEZ SALGADO; CARLOS VEGA DE LAS HERAS. Melting point and phase diagram of methanol as obtained from computer simulations of the OPLS model. Journal of Chemical Physics. 132, pp. 094505 - 094505. (United States of America): 01/03/2010. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Source of citations: WOS **Citations:** 10
- 118** CARLOS VEGA DE LAS HERAS; M. M. Conde; C. McBride; J. L. F. Abascal; E. G. Noya; R. RAMIREZ; L. M. Sese. Heat capacity of water: A signature of nuclear quantum effects. Journal of Chemical Physics. 132, pp. 046101 - 046101. (United States of America): 15/01/2010. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Total no. authors: 7
Source of citations: WOS **Citations:** 42
- 119** JOSE LUIS FERNANDEZ ABASCAL; EDUARDO SANZ; CARLOS VEGA DE LAS HERAS. Triple points and coexistence properties of the dense phases of water calculated using computer simulation. Physical Chemistry Chemical Physics. 11, pp. 556 - 562. (United Kingdom): 07/09/2009. ISSN 1463-9076
Type of production: Scientific paper **Format:** Journal
Position of signature: 3
Source of citations: WOS **Citations:** 14
- 120** E. G. Noya; R. RAMIREZ; L. M. Sese; CARLOS VEGA DE LAS HERAS. Quantum effects on the maximum in density of water as described by the TIP4PQ/2005 model. Journal of Chemical Physics. 131, pp. 124518 - 124518. (United States of America): 01/09/2009. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Source of citations: WOS **Citations:** 24

- 121** MARIA MARTIN CONDE; BEN SLATER; G TRIBELLO; CARLOS VEGA DE LAS HERAS. The phase diagram of water at negative pressures: Virtual ices. Journal of Chemical Physics. 131, pp. 034510 - 034510. (United States of America): 12/08/2009. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Position of signature: 2

Source of citations: WOS

Citations: 27

- 122** J. L. Aragonés; CARLOS VEGA DE LAS HERAS. Plastic crystal phases of simple water models. Journal of Chemical Physics. 130, pp. 244504 - 244504. (United States of America): 11/08/2009. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Position of signature: 2

Source of citations: WOS

Citations: 16

- 123** JOSE LUIS FERNANDEZ ABASCAL; JUAN LUIS ARAGONES GOMEZ; MIGUEL ANGEL GONZALEZ GONZALEZ; CARL MCBRIDE; EVA GONZALEZ NOYA; HELENA PI; CARLOS VEGA DE LAS HERAS. Anomalies in water as obtained from computer simulations of the TIP4P/2005 model: density maxima, and density, isothermal compressibility and heat capacity minima. Molecular Physics. 107, pp. 365 - 374. (United Kingdom): 06/06/2009. ISSN 0026-8976

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Format: Journal

Position of signature: 3

Source of citations: WOS

Citations: 74

- 124** CARL MCBRIDE; Eva G. Noya; RAFAEL RAMIREZ; LUIS M. SESE; CARLOS VEGA DE LAS HERAS. Quantum contributions in the ice phases: The path to a new empirical model for water-TIP4PQ/2005. Journal of Chemical Physics. 131, pp. 024506 - 024506. (United States of America): 01/06/2009. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Position of signature: 2

Source of citations: WOS

Citations: 46

- 125** JUAN LUIS ARAGONES GOMEZ; MARIA MARTIN CONDE; EVA GONZALEZ NOYA; CARLOS VEGA DE LAS HERAS. The phase diagram of water at high pressures as obtained by computer simulations of the TIP4P/2005 model: the appearance of a plastic crystal phase. Physical Chemistry Chemical Physics. 11, pp. 543 - 555. (United Kingdom): 30/01/2009. ISSN 1463-9076

Type of production: Scientific paper

Format: Journal

Position of signature: 4

Impact source: ISI

Impact index in year of publication: 3,5

Source of citations: WOS

Citations: 23

- 126** J.L.F. Abascal; J.L. Aragonés; M.M. Conde; C. Vega. What ice can teach us about water interactions: a critical comparison of the performance of different water models. Faraday Discussions. 141, pp. 251 - 276. (United Kingdom): 15/01/2009. ISSN 1359-6640

Type of production: Scientific paper

Format: Journal

Position of signature: 1

Impact source: ISI

Impact index in year of publication: 5,5

Source of citations: WOS

Citations: 177



Relevant publication: No

- 127** MARIA MARTIN CONDE; EVA GONZALEZ NOYA; CARLOS VEGA DE LAS HERAS. Computing the free energy of molecular solids by the Einstein molecule approach: Ices XIII and XIV, hard-dumbbells and a patchy model of proteins. Journal of Chemical Physics. pp. 104704 - 104704. (United States of America): 16/09/2008. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Position of signature: 3

Source of citations: WOS

Citations: 28

- 128** F GAMEZ; SANTIAGO LAGO ARANDA; P J MERKLIN; CARLOS VEGA DE LAS HERAS. Vapour-liquid equilibrium of fluids composed by oblate molecules. Molecular Physics. 106, pp. 1331 - 1339. (United Kingdom): 01/08/2008. ISSN 0026-8976

Type of production: Scientific paper

Format: Journal

Position of signature: 4

Source of citations: WOS

Citations: 8

- 129** MARIA MARTIN CONDE; ANDREJ PATRYKIEJEV; CARLOS VEGA DE LAS HERAS. The thickness of a liquid layer on the free surface of ice as obtained from computer simulation. Journal of Chemical Physics. 129, pp. 014702 - 014702. (United States of America): 15/07/2008. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Position of signature: 2

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Impact index in year of publication: 3,33

Source of citations: WOS

Citations: 47

- 130** ENRIQUE DE MIGUEL; EVA GONZALEZ NOYA; CARLOS VEGA DE LAS HERAS. Determination of the melting point of hard spheres from direct coexistence simulation methods. Journal of Chemical Physics. 128, pp. 154507 - 154507. (United States of America): 16/04/2008. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Position of signature: 2

Impact source: ISI

Impact index in year of publication: 3,33

Source of citations: WOS

Citations: 38

- 131** JOSE LUIS FERNANDEZ ABASCAL; EVA GONZALEZ NOYA; EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. Determination of phase diagrams via computer simulation: methodology and applications to water, electrolytes and proteins. Journal of Physics Condensed Matter. 20, pp. 153101 - 153101. (United Kingdom): 15/04/2008. ISSN 0953-8984

Type of production: Scientific paper

Format: Journal

Position of signature: 1

Impact source: ISI

Impact index in year of publication: 2,5

Source of citations: WOS

Citations: 127

- 132** JOSE LUIS FERNANDEZ ABASCAL; CARLOS VEGA DE LAS HERAS. The Water Forcefield: Importance of Dipolar and Quadrupolar Interactions. Journal of Physical Chemistry C. 111, pp. 15811 - 15822. (United States of America): 01/11/2007. ISSN 1932-7447

Type of production: Scientific paper

Format: Journal



Position of signature: 2

Impact source: ISI

Impact index in year of publication: 4,0

Source of citations: WOS

Citations: 27

- 133** JUAN LUIS ARAGONES GOMEZ; CARLOS MENDUIÑA FERNANDEZ; EVA GONZALEZ NOYA; CARLOS VEGA DE LAS HERAS. Equation of state, thermal expansion coefficient and isothermal compressibility for ices Ih, II, III, V and VI, as obtained from computer simulation. Journal of Physical Chemistry C. 11, pp. 15877 - 15888. (United States of America): 16/10/2007. ISSN 1932-7447

Type of production: Scientific paper

Format: Journal

Position of signature: 3

Impact source: ISI

Impact index in year of publication: 4,5

Source of citations: WOS

Citations: 24

- 134** JOSE LUIS FERNANDEZ ABASCAL; JUAN LUIS ARAGONES GOMEZ; EVA GONZALEZ NOYA; CARLOS VEGA DE LAS HERAS. Properties of ices at 0 K: A test of water models. Journal of Chemical Physics. 127, pp. 154518 - 154518. (United States of America): 15/10/2007. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Position of signature: 4

Source of citations: WOS

Citations: 28

- 135** EVA GONZALEZ NOYA; CARLOS VEGA DE LAS HERAS. Revisiting the Frenkel-Ladd method to compute the free energy of solids: the Einstein molecule approach. Journal of Chemical Physics. 127, pp. 154113 - 154113. (United States of America): 15/10/2007. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Position of signature: 1

Impact source: ISI

Impact index in year of publication: 3,33

Source of citations: WOS

Citations: 62

- 136** J. L. F. Abascal; R. Garcia Fernandez; L. G. MacDowell; E. SANZ; CARLOS VEGA DE LAS HERAS. Ice: A fruitful source of information about liquid water, volumen 136, Impacto 1,7 , 9 citas. Journal of Molecular Liquids. 136, pp. 214 - 220. (Holland): 29/09/2007. ISSN 0167-7322

Type of production: Scientific paper

Format: Journal

Position of signature: 5

Source of citations: WOS

Citations: 9

- 137** JOSE LUIS FERNANDEZ ABASCAL; CARLOS VEGA DE LAS HERAS. The melting point of hexagonal ice (Ih) is strongly dependent on the quadrupole of the water models. Physical Chemistry Chemical Physics. 9, pp. 2775 - 2778. (United Kingdom): 01/09/2007. ISSN 1463-9076

Type of production: Scientific paper

Format: Journal

Position of signature: 2

Source of citations: WOS

Citations: 23

- 138** H. Docherty; A. GALINDO; E. SANZ; CARLOS VEGA DE LAS HERAS. Investigation of the salting out of methane from aqueous electrolyte solutions using computer simulations, volumen 111, Impacto 3,8 , 16 citas. Journal of Physical Chemistry B. 11, pp. 8993 - 9000. (United States of America): 21/08/2007. ISSN 1520-6106



Type of production: Scientific paper
Position of signature: 4
Impact source: ISI
Impact index in year of publication: 4,0

Format: Journal

Source of citations: WOS

Citations: 17

- 139** JPK DOYE; EVA GONZALEZ NOYA; A A LOUIS; CARLOS VEGA DE LAS HERAS. Phase diagram of model anisotropic particles with octahedral symmetry, volumen 127, 054501, 38 citas. Journal of Chemical Physics. 127, pp. 054501 - 054501. (United States of America): 15/08/2007. ISSN 0021-9606

Type of production: Scientific paper
Position of signature: 2
Impact source: ISI
Impact index in year of publication: 3,33

Format: Journal

Source of citations: WOS

Citations: 56

- 140** Jose B. Caballero; Eva G. Noya; CARLOS VEGA DE LAS HERAS. Complete phase behavior of the symmetrical colloidal electrolyte, volumen 127, 244910, Impacto 3,33, 5 citas,. Journal of Chemical Physics. 127, pp. 244910 - 244910. (United States of America): 25/07/2007. ISSN 0021-9606

Type of production: Scientific paper
Position of signature: 3

Format: Journal

- 141** JOSE LUIS FERNANDEZ ABASCAL; CARLOS VEGA DE LAS HERAS. Dipole-quadrupole force ratios determine the ability of potential models to describe the phase diagram of water. Physical Review Letters. 98, pp. 237801 - 237801. (United States of America): 01/07/2007. ISSN 0031-9007

Type of production: Scientific paper
Position of signature: 2
Impact source: ISI
Impact index in year of publication: 7,5

Format: Journal

Source of citations: WOS

Citations: 37

- 142** C. Vega; E. de Miguel. The surface tension of the most popular models of water by using the extended Widom method. Journal of Chemical Physics. 126, pp. 154707 - 154707. (United States of America): 15/04/2007. ISSN 0021-9606

Type of production: Scientific paper
Position of signature: 1
Impact source: ISI
Impact index in year of publication: 3,33

Format: Journal

Source of citations: WOS

Citations: 227

Relevant publication: No

- 143** EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. Solubility of KF and NaCl in water by molecular simulation. Journal of Chemical Physics. 126, pp. 014507 - 014507. (United States of America): 15/01/2007. ISSN 0021-9606

Type of production: Scientific paper
Position of signature: 2
Impact source: ISI
Impact index in year of publication: 3,33

Format: Journal

Source of citations: WOS

Citations: 49

- 144** MARIA MARTIN CONDE; A PATRYKIEJEV; CARLOS VEGA DE LAS HERAS. Absence of superheating for ice Ih with a free surface: a new method of determining the melting point of different water models, volumen 104, Impacto 1,8, 28 citas. Molecular Physics. 104, pp. 3583 - 3592. (United Kingdom): 20/12/2006. ISSN 0026-8976
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Impact source: ISI
Impact index in year of publication: 1,7
Source of citations: WOS **Citations:** 36
- 145** JOSE LUIS FERNANDEZ ABASCAL; IVO NEZBEDA; CARLOS VEGA DE LAS HERAS. Vapor-liquid equilibria from the triple point up to the critical point for the new generation of TIP4P like models: TIP4P/Ew, TIP4P/2005 and TIP4P/Ice, volumen 125, 034503, impacto 3,33,61 citas. Journal of Chemical Physics. 125, pp. 034503 - 034503. (United States of America): 08/08/2006. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 97
- 146** LUIS GONZALEZ MAC-DOWELL; MARIA MARTIN CONDE; CARLOS VEGA DE LAS HERAS. Computer simulation of two new solid phases of water: ice XIII and ice XIV, volumen 125, 116101, impacto 3,33,9 citas. Journal of Chemical Physics. 125, pp. 116101 - 116101. (United States of America): 01/08/2006. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Source of citations: WOS **Citations:** 9
- 147** JOSE LUIS FERNANDEZ ABASCAL; MARCELO CARIGNANO; RAMON GARCIA FERNANDEZ; CARLOS VEGA DE LAS HERAS. The melting temperature of the six site potential model of water, volumen 125, 166101, Impacto 3,33,43 citas. Journal of Chemical Physics. 125, pp. 166101 - 166101. (United States of America): 01/08/2006. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 3
Source of citations: WOS **Citations:** 52
- 148** H DOCHERTY; A GALINDO; EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. A potential model for methane in water describing correctly the solubility of the gas and the properties of the methane hydrate, volumen 125, 074510, Impacto 3,33,46 citas. Journal of Chemical Physics. 125, pp. 074510 - 074510. (United States of America): 15/07/2006. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 3
Source of citations: WOS **Citations:** 66
- 149** JOSE LUIS FERNANDEZ ABASCAL; RAMON GARCIA FERNANDEZ; CARLOS VEGA DE LAS HERAS. The melting point of ice Ih for common water models calculated from direct coexistence of the solid-liquid interface, volumen 124, 144506, impacto 3,33,120 citas. Journal of Chemical Physics. 124, pp. 144506 - 144506. (United States of America): 01/04/2006. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 3
Source of citations: WOS **Citations:** 181



- 150** JOSE LUIS FERNANDEZ ABASCAL; CARLOS VEGA DE LAS HERAS. A general purpose model for the condensed phases of water: TIP4P/2005,volumen 123,234505,impacto 3,33,360 citas. Journal of Chemical Physics. 123, pp. 234505 - 234505. (United States of America): 20/12/2005. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Position of signature: 2

Impact source: ISI

Impact index in year of publication: 3,33

Source of citations: WOS

Citations: 757

- 151** JOSE LUIS FERNANDEZ ABASCAL; CARLOS VEGA DE LAS HERAS. Relation between the melting temperature and the temperature of maximum density for the most common models of water,volumen 123,144504,impacto 3,33,60 citas. Journal of Chemical Physics. 123, pp. 144504 - 144504. (United States of America): 01/09/2005. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Position of signature: 1

Source of citations: WOS

Citations: 81

- 152** JOSE LUIS FERNANDEZ ABASCAL; RAMON GARCIA FERNANDEZ; EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. A potential model for the study of ices and amorphous water: TIP4P/Ice,volumen 122,234511,impacto 3,33,155 citas. Journal of Chemical Physics. 122, pp. 234511 - 234511. (United States of America): 01/07/2005. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Position of signature: 4

Source of citations: WOS

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- 153** CARL MCBRIDE; EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. Non-Markovian melting: A novel procedure to generate initial liquid like phases for small molecules for use in computer simulation studies. Computer Physics Communications. 170, pp. 137 - 143. (Holland): 18/05/2005. ISSN 0010-4655

Type of production: Scientific paper

Format: Journal

Position of signature: 3

Impact source: ISI

Impact index in year of publication: 3,5

- 154** JOSE LUIS FERNANDEZ ABASCAL; LUIS GONZALEZ MAC-DOWELL; CARL MCBRIDE; EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. Can simple models describe the phase diagram of water?,volumen 17, impacto 2,5,45 citas. Journal of Physics Condensed Matter. pp. 3265 - 3272. (United Kingdom): 01/04/2005. ISSN 0953-8984

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Format: Journal

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Citations: 52

- 155** JOSE LUIS FERNANDEZ ABASCAL; CARL MCBRIDE; EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. Radial distribution functions and densities for SPC/E, TIP4P and TIP5P models for liquid water and ices Ih, Ic, II, III, IV, V, VI, VII, VIII, IX, XI and XII,volumen 7,impacto 3,7,47 citas. Physical Chemistry Chemical Physics. 7, pp. 1450 - 1456. (United Kingdom): 02/03/2005. ISSN 1463-9076

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Source of citations: WOS

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- 156** JOSE LUIS FERNANDEZ ABASCAL; EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. The melting temperature of the most popular models of water, volumen 122, 114507, impacto 3,33, 171 citas. Journal of Chemical Physics. 122, pp. 114507 - 114507. (United States of America): 01/03/2005. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 208
- 157** JOSE LUIS FERNANDEZ ABASCAL; LUIS GONZALEZ MAC-DOWELL; CARL MCBRIDE; EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. The range of metastability of ice-water melting for two simple models of water. Molecular Physics. 103, pp. 1 - 5. (United Kingdom): 01/02/2005. ISSN 0026-8976
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Source of citations: WOS **Citations:** 43
- 158** F.J. BLAS; A. GALINDO; EDUARDO SANZ GARCIA; LUIS GONZALEZ MAC-DOWELL; CARLOS VEGA DE LAS HERAS. Computer simulation study of the global phase behavior of linear rigid Lennard-Jones chain molecules: Comparison with flexible models. Journal of Chemical Physics. 120, pp. 3957 - 3968. (United States of America): 31/12/2004. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 5
Impact source: ISI
Impact index in year of publication: 3,33
Source of citations: WOS **Citations:** 14
- 159** F.J. BLAS; EDUARDO SANZ GARCIA; LUIS GONZALEZ MAC-DOWELL; CARLOS VEGA DE LAS HERAS. Molecular modeling of flexible molecules: vapor-liquid and fluid solid equilibria. Journal of Molecular Liquids. 113, pp. 37 - 51. (Holland): 31/12/2004. ISSN 0167-7322
Type of production: Scientific paper **Format:** Journal
Position of signature: 4
Impact source: ISI
Impact index in year of publication: 1,6
Source of citations: WOS **Citations:** 10
- 160** JOSE LUIS FERNANDEZ ABASCAL; CARL MCBRIDE; EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. Formation of high density amorphous ice by decompression of ice VII and ice VIII at 135 K. Journal of Chemical Physics. 121, pp. 11907 - 11911. (United States of America): 01/10/2004. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Source of citations: WOS **Citations:** 21
- 161** JOSE LUIS FERNANDEZ ABASCAL; LUIS GONZALEZ MAC-DOWELL; EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. Combinatorial entropy and phase diagram of partially ordered ice phases. Journal of Chemical Physics. 121, pp. 10145 - 10158. (United States of America): 01/09/2004. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 3
Source of citations: WOS **Citations:** 42

- 162** JOSE LUIS FERNANDEZ ABASCAL; LUIS GONZALEZ MAC-DOWELL; EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. Phase diagram of water from computer simulation. Physical Review Letters. 92, pp. 255701 - 255701. (United States of America): 01/07/2004. ISSN 0031-9007

Type of production: Scientific paper

Format: Journal

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Impact source: ISI

Impact index in year of publication: 7,5

Source of citations: WOS

Citations: 177

- 163** JOSE LUIS FERNANDEZ ABASCAL; LUIS GONZALEZ MAC-DOWELL; EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. Tracing the phase diagram of the TIP4P model of water. Journal of Chemical Physics. 121, pp. 1165 - 1166. (United States of America): 01/07/2004. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Position of signature: 2

Source of citations: WOS

Citations: 62

- 164** F.J. BLAS; A. GALINDO; CARLOS VEGA DE LAS HERAS. Study of the solid-liquid-vapor phase equilibria of flexible chain molecules using Wertheim's thermodynamic perturbation theory. Molecular Physics. pp. 449 - 458. (United Kingdom): 31/12/2003. ISSN 0026-8976

Type of production: Scientific paper

Format: Journal

Position of signature: 2

Source of citations: WOS

Citations: 16

- 165** F.J. BLAS; A. GALINDO; CARL MCBRIDE; E. DE MIGUEL; CARLOS VEGA DE LAS HERAS. The phase diagram of the two center Lennard-Jones model as obtained from computer simulation and from Wertheim's thermodynamic perturbation theory. Journal of Chemical Physics. 118, pp. 10696 - 10706. (United States of America): 31/12/2003. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

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Impact source: ISI

Impact index in year of publication: 3,33

Source of citations: WOS

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- 166** CARL MCBRIDE; EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. The properties of fully flexible Lennard-Jones chains in the solid phase: Wertheim's TPT1 theory and simulation. Molecular Physics. pp. 2241 - 2255. (United Kingdom): 31/12/2003. ISSN 0026-8976

Type of production: Scientific paper

Format: Journal

Position of signature: 4

Source of citations: WOS

Citations: 12

- 167** E. DE MIGUEL; LUIS GONZALEZ MAC-DOWELL; CARLOS MENDUIÑA FERNANDEZ; CARLOS VEGA DE LAS HERAS. The third virial coefficient and critical properties of quadrupolar two center Lennard-Jones models. Physical Chemistry Chemical Physics. pp. 2851 - 2857. (United Kingdom): 31/12/2003. ISSN 1463-9076

Type of production: Scientific paper

Format: Journal

Position of signature: 3

Source of citations: WOS

Citations: 10

- 168** JOSE LUIS FERNANDEZ ABASCAL; FERNANDO BRESME; CARL MCBRIDE; CARLOS VEGA DE LAS HERAS. Characterization of the order-disorder transition of a charged hard sphere model. *Physical Review E - Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics*. 68, pp. 525011 - 525014. (United States of America): 30/11/2003. ISSN 1063-651X
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Impact source: ISI
Impact index in year of publication: 2,3
Source of citations: WOS **Citations:** 6
- 169** LUIS GONZALEZ MAC-DOWELL; J. LARGO; M.J. MAESO; J.R. SOLANA; CARLOS VEGA DE LAS HERAS. Bonded hard-sphere theory and computer simulation of the equation of state of linear fused hard sphere fluids. *Journal of Chemical Physics*. 119, pp. 9633 - 9639. (United States of America): 01/10/2003. ISSN 0021-9606
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Position of signature: 1
Source of citations: WOS **Citations:** 8
- 170** E. DE MIGUEL; LUIS GONZALEZ MAC-DOWELL; CARLOS MENDUIÑA FERNANDEZ; CARLOS VEGA DE LAS HERAS. Critical properties of molecular fluids from the virial expansion. *Journal of Chemical Physics*. pp. 11367 - 11373. (United States of America): 15/07/2003. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 3
Source of citations: WOS **Citations:** 14
- 171** JOSE LUIS FERNANDEZ ABASCAL; FERNANDO BRESME; CARL MCBRIDE; CARLOS VEGA DE LAS HERAS. The fluid-solid equilibrium for a charged hard sphere model revisited. *Journal of Chemical Physics*. 119, pp. 964 - 971. (United States of America): 01/07/2003. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 47
- 172** F.J. BLAS; A. GALINDO; EDUARDO SANZ GARCIA; CARLOS VEGA DE LAS HERAS. Fluid-solid equilibria of flexible and linear rigid tangent chains from Wertheim's thermodynamic perturbation theory. *Journal of Chemical Physics*. 119, pp. 10958 - 10971. (United States of America): 01/03/2003. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 3
Source of citations: WOS **Citations:** 14
- 173** CARL MCBRIDE; CARLOS VEGA DE LAS HERAS. A MONTE CARLO STUDY OF THE INFLUENCE OF MOLECULAR FLEXIBILITY ON THE PHASE DIAGRAM OF A FUSED HARD SPHERE MODEL. *Journal of Chemical Physics*. pp. 10370 - 10379. (United States of America): 01/09/2002. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 27
- 174** E. DE MIGUEL; CARLOS VEGA DE LAS HERAS. THE GLOBAL PHASE DIAGRAM OF THE GAY BERNE MODEL, volumen 117, impacto 3,33, 54 citas. *Journal of Chemical Physics*. 117, pp. 6313 - 6322. (United States of America): 01/08/2002. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal

**Position of signature:** 1**Source of citations:** WOS**Citations:** 60

- 175** LUIS GONZALEZ MAC-DOWELL; CARL MCBRIDE; CARLOS VEGA DE LAS HERAS. THE EFFECT OF FLEXIBILITY ON THE PHASE DIAGRAM OF SIMPLE MOLECULAR MODELS. *Physical Chemistry Chemical Physics*. 4, pp. 853 - 862. (United Kingdom): 01/07/2002. ISSN 1463-9076

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- 176** CARL MCBRIDE; CARLOS VEGA DE LAS HERAS. FLUID-SOLID EQUILIBRIUM FOR TWO DIMENSIONAL HARD DISK CHAINS FROM WERTHEIM'S PERTURBATION THEORY. *Journal of Chemical Physics*. 116, pp. 1757 - 1759. (United States of America): 01/06/2002. ISSN 0021-9606

Type of production: Scientific paper**Format:** Journal**Position of signature:** 1**Source of citations:** WOS**Citations:** 22

- 177** CARL MCBRIDE; CARLOS MENDUIÑA FERNANDEZ; CARLOS VEGA DE LAS HERAS. THE SECOND VIRIAL COEFFICIENT OF THE DIPOLEAR TWO CENTER LENNARD-JONES MODEL. *Physical Chemistry Chemical Physics*. 4, pp. 3000 - 3007. (United Kingdom): 01/06/2002. ISSN 1463-9076

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- 178** CARL MCBRIDE; CARLOS VEGA DE LAS HERAS. SCALING LAWS FOR THE EQUATION OF STATE OF FLEXIBLE AND LINEAR TANGENT HARD SPHERE CHAINS. *Physical Review E - Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics*. pp. 052501 - 052501. (United States of America): 03/05/2002. ISSN 1063-651X

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- 179** LUIS GONZALEZ MAC-DOWELL; J. LARGO; CARLOS VEGA DE LAS HERAS. A COMPUTER SIMULATION STUDY OF RACEMIC MIXTURES. *Molecular Physics*. 100, pp. 2397 - 2415. (United Kingdom): 01/04/2002. ISSN 0026-8976

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- 181** LG MacDowell; C McBride; CARLOS VEGA DE LAS HERAS. Liquid crystal phase formation for the linear tangent hard sphere model from Monte Carlo simulations, volumen 115, impacto 3,33, 29 citas. *Journal of Chemical Physics*. 115, pp. 4203 - 4211. (United States of America): 14/12/2001. ISSN 0021-9606

**Type of production:** Scientific paper**Format:** Journal**Position of signature:** 1**Source of citations:** WOS**Citations:** 41

- 182** LG MacDowell; E SANZ; CARLOS VEGA DE LAS HERAS. Equation of state of model branched alkanes: Theoretical predictions and configurational bias Monte Carlo simulations. Journal of Chemical Physics. 115, pp. 6220 - 6235. (United States of America): 22/10/2001. ISSN 0021-9606

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Type of production: Scientific paper**Format:** Journal**Position of signature:** 1**Source of citations:** WOS**Citations:** 47

- 184** C Menduina; C McBride; CARLOS VEGA DE LAS HERAS. The second virial coefficient of quadrupolar two center Lennard-Jones models. Physical Chemistry Chemical Physics. 3, pp. 1289 - 1296. (United Kingdom): 04/05/2001. ISSN 1463-9076

Type of production: Scientific paper**Format:** Journal**Position of signature:** 3**Source of citations:** WOS**Citations:** 18

- 185** LG MacDowell; C McBride; CARLOS VEGA DE LAS HERAS. Isotropic-nematic phase transition: Influence of intramolecular flexibility using a fused hard sphere model, volumen 64, 011703, 33 citas. Physical Review E - Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics. 64, pp. 011703 - 011703. (United States of America): 02/04/2001. ISSN 1063-651X

Type of production: Scientific paper**Format:** Journal**Position of signature:** 2**Source of citations:** WOS**Citations:** 42

- 186** CARLOS VEGA DE LAS HERAS. Evaluating virial coefficients for multicomponent mixtures: hard sphere mixtures and flexible chains. Molecular Physics. 98, pp. 973 - 985. (United Kingdom): 30/11/2000. ISSN 0026-8976

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- 187** LG MacDowell; CARLOS VEGA DE LAS HERAS. Critical temperature of infinitely long chains from Wertheim's perturbation theory. Molecular Physics. 98, pp. 1295 - 1308. (United Kingdom): 01/09/2000. ISSN 0026-8976

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Position of signature: 1
Impact source: ISI
Impact index in year of publication: 3,33
Source of citations: WOS **Citations:** 25
- 189** A.P. Malanoski; C. Vega; P.A. Monson. An application of Cell Theory to Molecular Models of n-alkane solids. Molecular Physics. 98, pp. 363 - 370. 15/05/2000.
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- 190** JOSE LUIS FERNANDEZ ABASCAL; F BRESME; CARLOS VEGA DE LAS HERAS. Order-disorder transition in the solid phase of a charged hard sphere model,volumen 85, impacto 7,5,43 citas. Physical Review Letters. 85, pp. 3217 - 3220. (United States of America): 01/05/2000. ISSN 0031-9007
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Source of citations: WOS **Citations:** 43
- 191** L. G. MacDowell; M Muller; CARLOS VEGA DE LAS HERAS; K Binder. Equation of state and critical behavior of polymer models: A quantitative comparison between Wertheim's thermodynamic perturbation theory and computer simulations. Journal of Chemical Physics. 113, pp. 419 - 433. (United States of America): 22/04/2000. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 3
Source of citations: WOS **Citations:** 60
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Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 9
- 193** JUAN J. FREIRE; ANTONIO LOPEZ RODRIGUEZ; CARLOS VEGA DE LAS HERAS. Determination of potential parameters for alkanes. Journal of Chemical Physics. 111, pp. 438 - 439. (United States of America): 04/11/1999. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Source of citations: WOS **Citations:** 6
- 194** L. G. MacDowell; CARLOS VEGA DE LAS HERAS; ANTONIO LOPEZ RODRIGUEZ. Critical properties of mixtures of alkanes from perturbation theory. Journal of Chemical Physics. 111, pp. 3183 - 3191. (United States of America): 03/06/1999. ISSN 0021-9606
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Source of citations: WOS **Citations:** 5



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Source of citations: WOS

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Source of citations: WOS

Citations: 13

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Position of signature: 1

Impact source: ISI

Impact index in year of publication: 1,5

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Position of signature: 4
Source of citations: WOS **Citations:** 16
- 203** S. calero; Benito Garzon; SANTIAGO LAGO ARANDA; CARLOS VEGA DE LAS HERAS. Accurate simulations of the vapor-liquid equilibrium of important organic solvents and other diatomics. Journal of Physical Chemistry B. 101, pp. 6763 - 6771. (United States of America): 08/08/1997. ISSN 1520-6106
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Source of citations: WOS **Citations:** 24
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Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 43
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Position of signature: 2
Source of citations: WOS **Citations:** 16
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Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 16
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Position of signature: 3
Source of citations: WOS **Citations:** 14
- 208** JOSE LUIS FERNANDEZ ABASCAL; FERNANDO BRESME; CARLOS VEGA DE LAS HERAS. Fluid-solid equilibrium of a charged hard-sphere model. Physical Review E - Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics. 54, pp. 2746 - 2760. (United States of America): 01/10/1996. ISSN 1063-651X
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 42



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Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 19
- 210** L. G. MacDowell; P. PADILLA; CARLOS VEGA DE LAS HERAS. Equation of state for hard n-alkane models: Long chains. *Journal of Chemical Physics*. 104, pp. 701 - 713. (United States of America): 01/06/1996. ISSN 0021-9606
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Position of signature: 1
Source of citations: WOS **Citations:** 24
- 211** CARLOS VEGA DE LAS HERAS; Benito Garzon; L. G. MacDowell; S. calero; SANTIAGO LAGO ARANDA; P. PADILLA. The vapour-liquid equilibrium of n-alkanes. *Journal of Physics Condensed Matter*. 8, pp. 9643 - 9648. (United Kingdom): 05/05/1996. ISSN 0953-8984
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Position of signature: 1
- 212** ANTONIO LOPEZ RODRIGUEZ; CARLOS VEGA DE LAS HERAS. Second virial coefficients, critical temperatures, and the molecular shapes of long n-alkanes. *Journal of Chemical Physics*. 105, pp. 4223 - 4233. (United States of America): 04/04/1996. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 17
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Position of signature: 2
Source of citations: WOS **Citations:** 7
- 214** X. Cottin; P. A. Monson; E.P.A. Paras; CARLOS VEGA DE LAS HERAS. Solid-fluid equilibrium: New perspectives from molecular theory. *Fluid Phase Equilibria*. 117, pp. 114 - 125. (Holland): 01/01/1996. ISSN 0378-3812
Type of production: Scientific paper **Format:** Journal
Position of signature: 3
Source of citations: WOS **Citations:** 12
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Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 16
- 216** Fernando delRio; Alejandro Gil-Villegas; A Malijevsky; CARLOS VEGA DE LAS HERAS. STRUCTURE OF VARIABLE-WIDTH SQUARE-WELL FLUIDS FROM THE REFERENCE HYPERNETTED-CHAIN EQUATION. *Molecular Physics*. 86, pp. 857 - 864. (United Kingdom): 06/09/1995. ISSN 0026-8976
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Position of signature: 3

**Source of citations:** WOS**Citations:** 11

- 217** P. PADILLA; CARLOS VEGA DE LAS HERAS. PACKING EFFECTS ON THE CONFORMATIONAL EQUILIBRIUM OF ALKANES. *Molecular Physics*. 84, pp. 435 - 450. (United Kingdom): 21/08/1995. ISSN 0026-8976

Type of production: Scientific paper**Format:** Journal**Position of signature:** 2**Source of citations:** WOS**Citations:** 17

- 218** Benito Garzon; SANTIAGO LAGO ARANDA; L.F. Rull; CARLOS VEGA DE LAS HERAS. COMPUTER-SIMULATION OF VAPOR-LIQUID-EQUILIBRIA OF LINEAR DIPOLAR FLUIDS - DEPARTURES FROM THE PRINCIPLE OF CORRESPONDING STATES. *Journal of Chemical Physics*. 102, pp. 7204 - 7215. (United States of America): 01/07/1995. ISSN 0021-9606

Type of production: Scientific paper**Format:** Journal**Position of signature:** 3**Source of citations:** WOS**Citations:** 23

- 219** Benito Garzon; SANTIAGO LAGO ARANDA; L. G. MacDowell; CARLOS VEGA DE LAS HERAS. VAPOR-LIQUID-EQUILIBRIA OF PROPANE AND N-ALKANE CONFORMERS. *Molecular Physics*. 85, pp. 679 - 699. (United Kingdom): 01/07/1995. ISSN 0026-8976

Type of production: Scientific paper**Format:** Journal**Position of signature:** 1

- 220** SANTIAGO LAGO ARANDA; L.F. Rull; CARLOS VEGA DE LAS HERAS. LOCATION OF THE FISHER-WIDOM LINE FOR SYSTEMS INTERACTING THROUGH SHORT-RANGED POTENTIALS. *Physical Review E - Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics*. 51, pp. 3146 - 3155. (United States of America): 01/06/1995. ISSN 1063-651X

Type of production: Scientific paper**Format:** Journal**Position of signature:** 1**Source of citations:** WOS**Citations:** 17

- 221** P. A. Monson; CARLOS VEGA DE LAS HERAS. SOLID-FLUID EQUILIBRIA FOR QUADRUPOLE HARD DUMBBELLS VIA MONTE-CARLO SIMULATION. *Journal of Chemical Physics*. 102, pp. 1361 - 1372. (United States of America): 01/03/1995. ISSN 0021-9606

Type of production: Scientific paper**Format:** Journal**Position of signature:** 1**Source of citations:** WOS**Citations:** 31

- 222** Benito Garzon; SANTIAGO LAGO ARANDA; CARLOS VEGA DE LAS HERAS. REACTION FIELD SIMULATIONS OF THE VAPOR-LIQUID-EQUILIBRIA OF DIPOLAR FLUIDS - DOES THE REACTION FIELD DIELECTRIC-CONSTANT AFFECT THE COEXISTENCE PROPERTIES. *Chemical Physics Letters*. 231, pp. 366 - 372. (Holland): 27/11/1994. ISSN 0009-2614

Type of production: Scientific paper**Format:** Journal**Position of signature:** 3**Source of citations:** WOS**Citations:** 34

- 223** Benito Garzon; SANTIAGO LAGO ARANDA; CARLOS VEGA DE LAS HERAS. LINEAR HARD-SPHERE MODELS - VIRIAL-COEFFICIENTS AND EQUATION OF STATE. *Molecular Physics*. 82, pp. 1233 - 1247. (United Kingdom): 07/09/1994. ISSN 0026-8976

Type of production: Scientific paper**Format:** Journal**Position of signature:** 1



Source of citations: WOS

Citations: 19

- 224** Benito Garzon; SANTIAGO LAGO ARANDA; J.L. LopezMartin; CARLOS VEGA DE LAS HERAS. VAPOR-LIQUID-EQUILIBRIUM OF PURE FLUIDS FROM A SIMPLE THERMODYNAMIC PERTURBATION-THEORY. Journal of Physical Chemistry. 98, pp. 5355 - 5361. (United States of America): 20/07/1994. ISSN 0022-3654

Type of production: Scientific paper

Format: Journal

Position of signature: 4

Source of citations: WOS

Citations: 4

- 225** SANTIAGO LAGO ARANDA; CARLOS VEGA DE LAS HERAS. A FAST ALGORITHM TO EVALUATE THE SHORTEST DISTANCE BETWEEN RODS. Computers and Chemistry. 18, pp. 55 - 59. (United Kingdom): 01/06/1994. ISSN 0097-8485

Type of production: Scientific paper

Format: Journal

Position of signature: 1

Source of citations: WOS

Citations: 42

- 226** Benito Garzon; SANTIAGO LAGO ARANDA; CARLOS VEGA DE LAS HERAS. LIQUID-VAPOR EQUILIBRIA OF POLAR FLUIDS FROM A VAN DER WAALS-LIKE THEORY. Journal of Physical Chemistry. 98, pp. 11181 - 11192. (United States of America): 01/05/1994. ISSN 0022-3654

Type of production: Scientific paper

Format: Journal

Position of signature: 1

Source of citations: WOS

Citations: 5

- 227** SANTIAGO LAGO ARANDA; CARLOS VEGA DE LAS HERAS. ISOTROPIC-NEMATIC TRANSITION OF HARD POLAR AND NONPOLAR MOLECULES. Journal of Chemical Physics. 100, pp. 6727 - 6737. (United States of America): 01/04/1994. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Position of signature: 1

Source of citations: WOS

Citations: 71

- 228** Benito Garzon; SANTIAGO LAGO ARANDA; CARLOS VEGA DE LAS HERAS. VIRIAL-COEFFICIENTS AND EQUATION OF STATE OF HARD ALKANE MODELS. Journal of Chemical Physics. 100, pp. 2182 - 2190. (United States of America): 01/04/1994. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Position of signature: 1

Source of citations: WOS

Citations: 44

- 229** Enrique deMiguel; Benito Garzon; SANTIAGO LAGO ARANDA; L.F. Rull; CARLOS VEGA DE LAS HERAS. COMPUTER-SIMULATION OF VAPOR-LIQUID-EQUILIBRIA OF LINEAR QUADRUPOLAR FLUIDS - DEPARTURES FROM THE PRINCIPLE OF CORRESPONDING STATES. Journal of Chemical Physics. 101, pp. 4166 - 4176. (United States of America): 22/02/1994. ISSN 0021-9606

Type of production: Scientific paper

Format: Journal

Position of signature: 3

Source of citations: WOS

Citations: 40

- 230** CARLOS VEGA DE LAS HERAS; R.D. Kaminski; P. A. Monson. ADSORPTION OF FLUIDS IN DISORDERED POROUS-MEDIA FROM INTEGRAL-EQUATION THEORY. Journal of Chemical Physics. pp. 3003 - 3013. (United States of America): 07/07/1993. ISSN 0021-9606

**Type of production:** Scientific paper**Format:** Journal**Position of signature:** 1**Source of citations:** WOS**Citations:** 93

- 231** P. A. Monson; E.P.A. Paras; CARLOS VEGA DE LAS HERAS. A GENERALIZED VAN-DER-WAALS THEORY OF SOLID FLUID EQUILIBRIA FOR NONSPHERICAL MOLECULES. *Molecular Physics*. 79, pp. 1063 - 1072. (United Kingdom): 01/07/1993. ISSN 0026-8976

Type of production: Scientific paper**Format:** Journal**Position of signature:** 2**Source of citations:** WOS**Citations:** 31

- 232** JUAN J. FREIRE; SANTIAGO LAGO ARANDA; ANTONIO LOPEZ RODRIGUEZ; CARLOS VEGA DE LAS HERAS. IMPROVED RESULTS FOR THE POTENTIAL PARAMETERS OF METHYL AND METHYLENE OBTAINED FROM 2ND VIRIAL-COEFFICIENTS OF N-ALKANES. *Molecular Physics*. 80, pp. 1565 - 1567. (United Kingdom): 01/07/1993. ISSN 0026-8976

Type of production: Scientific paper**Format:** Journal**Position of signature:** 2**Source of citations:** WOS**Citations:** 8

- 233** P. A. Monson; E.P.A. Paras; CARLOS VEGA DE LAS HERAS. ON THE STABILITY OF THE PLASTIC CRYSTAL PHASE OF HARD DUMBBELL SOLIDS. *Journal of Chemical Physics*. 97, pp. 8543 - 8548. (United States of America): 01/10/1992. ISSN 0021-9606

Type of production: Scientific paper**Format:** Journal**Position of signature:** 1**Source of citations:** WOS**Citations:** 60

- 234** S LABIK; SANTIAGO LAGO ARANDA; A Malijevsky; R POSPISIL; CARLOS VEGA DE LAS HERAS. THERMODYNAMIC PROPERTIES OF MIXTURES OF KIHARA MOLECULAR FLUIDS FROM PERTURBATION-THEORY. *Journal of Physical Chemistry*. 96, pp. 1895 - 1899. (United States of America): 01/10/1992. ISSN 0022-3654

Type of production: Scientific paper**Format:** Journal**Position of signature:** 1**Source of citations:** WOS**Citations:** 5

- 235** CARLOS VEGA DE LAS HERAS. A PERTURBATION-THEORY OF HARD QUADRUPOLEAR FLUIDS. *Molecular Physics*. 75, pp. 427 - 442. (United Kingdom): 01/09/1992. ISSN 0026-8976

Type of production: Scientific paper**Format:** Journal**Position of signature:** 1**Source of citations:** WOS**Citations:** 15

- 236** P. A. Monson; E.P.A. Paras; CARLOS VEGA DE LAS HERAS. APPLICATION OF CELL THEORY TO THE THERMODYNAMIC PROPERTIES OF HARD DUMBBELL SOLIDS. *Molecular Physics*. 77, pp. 803 - 821. (United Kingdom): 07/07/1992. ISSN 0026-8976

Type of production: Scientific paper**Format:** Journal**Position of signature:** 2**Source of citations:** WOS**Citations:** 35

- 237** CARLOS VEGA DE LAS HERAS; SANTIAGO LAGO ARANDA; Enrique deMiguel; L.F. Rull. LIQUID VAPOR EQUILIBRIA OF LINEAR KIHARA MOLECULES. Journal of Physical Chemistry. 96, pp. 7431 - 7437. (United States of America): 01/07/1992. ISSN 0022-3654
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 29
- 238** CARLOS VEGA DE LAS HERAS; E.P.A. Paras; P. A. Monson. SOLID-FLUID EQUILIBRIA FOR HARD DUMBBELLS VIA MONTE-CARLO SIMULATION. Journal of Chemical Physics. 96, pp. 9060 - 9072. (United States of America): 01/06/1992. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Impact source: ISI
Impact index in year of publication: 3,33
Source of citations: WOS **Citations:** 112
- 239** K.E. Gubbins; CARLOS VEGA DE LAS HERAS. MONTE-CARLO STUDY OF QUADRUPOLE KIHARA FLUIDS. Molecular Physics. 75, pp. 881 - 895. (United Kingdom): 01/04/1992. ISSN 0026-8976
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 19
- 240** SANTIAGO LAGO ARANDA; P. PADILLA; CARLOS VEGA DE LAS HERAS. THERMODYNAMIC PROPERTIES OF NONPOLAR MOLECULAR FLUIDS OF DIFFERENT GEOMETRIES FROM PERTURBATION-THEORY. Journal of Physical Chemistry. 96, pp. 1900 - 1905. (United States of America): 01/04/1992. ISSN 0022-3654
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 16
- 241** SANTIAGO LAGO ARANDA; CARLOS VEGA DE LAS HERAS. STRUCTURAL STUDY OF THE ANGLE-AVERAGED SOFT KIHARA POTENTIAL FOR LINEAR MOLECULAR-MODELS - A TEST OF PERTURBATION-THEORY. Molecular Physics. 72, pp. 215 - 228. (United Kingdom): 01/08/1991. ISSN 0026-8976
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 16
- 242** SANTIAGO LAGO ARANDA; CARLOS VEGA DE LAS HERAS. IMPROVED PERTURBATION-THEORY OF KIHARA FLUIDS. Chemical Physics Letters. 185, pp. 516 - 521. (Holland): 07/07/1991. ISSN 0009-2614
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 13
- 243** SANTIAGO LAGO ARANDA; P. PADILLA; CARLOS VEGA DE LAS HERAS. A BRIDGE BETWEEN FISCHER AND BOUBLIK THERMODYNAMIC PERTURBATION THEORIES - CALCULATING THERMODYNAMIC PROPERTIES OF PURE SUBSTANCES. Molecular Physics. 74, pp. 161 - 176. (United Kingdom): 01/07/1991. ISSN 0026-8976
Type of production: Scientific paper **Format:** Journal
Position of signature: 3
Source of citations: WOS **Citations:** 5



- 244** JUAN J. FREIRE; SANTIAGO LAGO ARANDA; ANTONIO LOPEZ RODRIGUEZ; CARLOS VEGA DE LAS HERAS. POTENTIAL PARAMETERS OF METHYL AND METHYLENE OBTAINED FROM 2ND VIRIAL-COEFFICIENTS OF N-ALKANES. *Molecular Physics*. 73, pp. 691 - 701. (United Kingdom): 01/07/1991. ISSN 0026-8976
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Source of citations: WOS **Citations:** 22
- 245** SANTIAGO LAGO ARANDA; P. PADILLA; MARIA PAZ SEVILLA SIERRA; CARLOS VEGA DE LAS HERAS. SOLUTION OF THE PERCUS-YEVICK EQUATION FOR LINEAR-MOLECULES INTERACTING THROUGH EITHER A KIHARA OR A SOFT REPULSIVE POTENTIAL. *Physics and Chemistry of Liquids*. 23, pp. 1 - 14. (United Kingdom): 01/07/1991. ISSN 0031-9104
Type of production: Scientific paper **Format:** Journal
Position of signature: 3
Source of citations: WOS **Citations:** 10
- 246** SANTIAGO LAGO ARANDA; CARLOS VEGA DE LAS HERAS. PERTURBATION-THEORY OF ANGULAR MOLECULES INTERACTING THROUGH THE KIHARA POTENTIAL. *Journal of Chemical Physics*. 94, pp. 310 - 320. (United States of America): 01/03/1991. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 21
- 247** TOMAS BOUBLIK; MATEO DIAZ PEÑA; SANTIAGO LAGO ARANDA; CARLOS VEGA DE LAS HERAS. QUADRUPOLEAR HARD GAUSSIAN-OVERLAP FLUID. *Molecular Physics*. 71, pp. 1193 - 1203. (United Kingdom): 01/10/1990. ISSN 0026-8976
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Source of citations: WOS **Citations:** 14
- 248** TOMAS BOUBLIK; MATEO DIAZ PEÑA; CARLOS VEGA DE LAS HERAS. Equation of state of chain molecules. *Journal of Chemical Physics*. 93, pp. 730 - 736. (United States of America): 07/07/1990. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 2
Impact source: ISI
Impact index in year of publication: 3,33
Source of citations: WOS **Citations:** 123
- 249** SANTIAGO LAGO ARANDA; CARLOS VEGA DE LAS HERAS. Molecular dynamics study of propane using two simple potential models. *Journal of Chemical Physics*. 93, pp. 8171 - 8179. (United States of America): 01/03/1990. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Source of citations: WOS **Citations:** 19
- 250** J FISCHER; B SAAGER; CARLOS VEGA DE LAS HERAS. Molecular dynamics studies for the new refrigerant R152a with simple model potentials. *Molecular Physics*. 68, pp. 1079 - 1093. (United Kingdom): 01/07/1989. ISSN 0026-8976
Type of production: Scientific paper **Format:** Journal

**Position of signature:** 1**Source of citations:** WOS**Citations:** 45

- 251** CARLOS VEGA DE LAS HERAS; Daan Frenkel. MONTE-CARLO STUDY OF ROD-LIKE MOLECULES - A TEST OF PERTURBATION-THEORY FOR THE KIHARA MODEL. *Molecular Physics*. 67, pp. 633 - 650. (United Kingdom): 01/05/1989. ISSN 0026-8976

Type of production: Scientific paper**Format:** Journal**Position of signature:** 1**Source of citations:** WOS**Citations:** 25

- 252** Lago, S.; CARLOS VEGA DE LAS HERAS. A GENERALIZATION FOR MIXTURES OF A FAST ALGORITHM TO CALCULATE SOME INTERMOLECULAR ORIENTATIONAL AVERAGES. *Computers and Chemistry*. 12, pp. 343 - 356. (United Kingdom): 01/10/1988. ISSN 0097-8485

Type of production: Scientific paper**Format:** Journal**Position of signature:** 1**Source of citations:** WOS**Citations:** 19

- 253** N di Pasquale; J Algaba; P Montero de Hijes; I S Burgos; A R Tejedro; S R Yeandel; F J Blas; R L Davidchack; J R Espinosa; C L Freeman; J Harding; B Laird; E Sanz; C Vega; L Rovigatti. Solid-liquid interfacial free energy from computer simulations: Challenges and recent advances. *Chemical Reviews*. 28/02/2025.

Type of production: Review**Total no. authors:** 15

- 254** Ceriotti M; Jensen L; Manolopoulos D; Martinez T; Reichman D.R.; Sciortino F; Sherrill C.D.; Shi Q; Vega C; Wang L.S.; Weiss E; Zhu X; Stein J; Lian T. 2021 JCP Emerging Investigator Special Collection. *Journal of Chemical Physics*. 158, pp. 060401. 14/02/2023.

Type of production: Bibliographic review**Total no. authors:** 14**Corresponding author:** No

- 255** Ceriotti M; Jensen L; Manolopoulos D; Martinez T; Michaelides A; Ogilvie J; Reichman D.R.; Shi Q; Straub J; Vega C; Wang L.S.; Weiss E; Zhu X; Stein J; Lian T. 2020 JCP Emerging Investigator Special Collection. *Journal of Chemical Physics*. 155, pp. 230401. 21/12/2021.

Type of production: Bibliographic review**Total no. authors:** 15**Corresponding author:** No

- 256** Ediger M.; Jensen L.; Manolopoulos D.; Martinez T; Michaelides A; Reichman D.R.; Sherrill C.D.; Shi Q; Straub J.; Vega C.; Wang L.S.; Brigham E.C.; Lian T. JCP Emerging Investigator Special Collection 2019. *Journal of Chemical Physics*. 153, pp. 110402. 21/09/2020.

Type of production: Bibliographic review**Total no. authors:** 13**Corresponding author:** No

- 257** Fernando Bresme; Eduardo Sanz; Erich A Muller; Jose Manuel Romero Enrique; Carlos Vega. On the contributions of Luis F. Rull and José Luis F. Abascal to the development of the school of statistical mechanics in Spain. *Molecular Physics*. 122, pp. e2431370. 16/11/2024.

Type of production: Preface Article**Total no. authors:** 5**Corresponding author:** No

- 258** O Pizio; A Patrykiewicz; C Vega; L Pusztai; Ja Illytskyi; T Patsahan; A Trokhymchuk. In memoriam: Stefan Sokołowski. *Condensed Matter Physics*. 27, pp. 37001. 24/09/2024.

Type of production: Memorial article**Total no. authors:** 7**Corresponding author:** No



- 259** Michaelides A.; Manolopoulos D.; Vega C.; Hamm P.; Chandler D.W.; Brigham E.C.; Lester M.. Editorial: The Future of Chemical Physics Conference 2016. Journal of Chemical Physics. 145, pp. 220401. 14/12/2016.

Type of production: Editorial

Total no. authors: 7

Corresponding author: No

Works submitted to national or international conferences

- 1** **Title of the work:** Simulation of electrolytes in water
Name of the conference: 12th Liquid Matter Conference
Type of event: Conference
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
Corresponding author: Yes
City of event: Mainz, Germany
Date of event: 22/09/2024
End date: 27/09/2024
Type of contribution: Scientific paper
- 2** **Title of the work:** Simulations of water and electrolyte solutions: where are we ?
Name of the conference: XIII Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design
Type of event: Conference
Type of participation: Participatory - Plenary **Reasons for participation:** Upon invitation session
City of event: Evora, Portugal
Date of event: 09/09/2024
End date: 12/09/2024
Type of contribution: Scientific paper
- 3** **Title of the work:** Modeling electrolytes in water : the Madrid-2019 force field
Name of the conference: MSL 2024 Symposium in Liquids
Type of event: Conference
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Fukuoka, Japan
Date of event: 05/07/2024
End date: 07/07/2024
Type of contribution: Scientific paper
- 4** **Title of the work:** Simulations of electrolytes in water
Name of the conference: Water X
Type of event: Conference
Type of participation: Participatory - oral communication
Corresponding author: Yes
City of event: La Maddalena, Italy
Date of event: 25/05/2024
End date: 30/05/2024
C. Vega; I.M. Zeron; J.L.F. Abascal; L.F. Sedano; E.G. Noya; C.P. Lamas; V.M. Trejos; M de Lucas; F Gamez; S Blazquez.



- 5** **Title of the work:** Fifty Years Simulating Water and Electrolyte Solutions : Where Are We?
Name of the conference: Charla plenaria invitada: Theoretical Chemistry Group , Universidad Cambridge
Type of participation: Participatory - Plenary session
City of event: Universidad de Cambridge,
Date of event: 01/11/2023
End date: 01/11/2023
City organizing entity: United Kingdom
- 6** **Title of the work:** Challenging the obvious answer for different questions concerning the Young-Laplace equation and the way we simulate electrolytes
Name of the conference: Cecam workshop: Challenges and opportunities in non-equilibrium soft matter, celebrating Daan Frenkel 75th birthday
Type of participation: Participatory - invited/keynote talk
City of event: Barcelona,
Date of event: 24/09/2023
End date: 27/09/2023
Organising entity: Cecam
- 7** **Title of the work:** Simulation studies of water and electrolyte aqueous solutions
Name of the conference: Charla plenaria invitada: Czech Academy of Sciences
Type of participation: Participatory - Plenary session
City of event: Praga,
Date of event: 23/06/2023
End date: 23/06/2023
City organizing entity: Institute of Organic Chemistry and Biochemistry. Czech Academy of Sciences., Czech Republic
- 8** **Title of the work:** Simulation Studies of Supercooled Water and Electrolyte Solutions
Name of the conference: Liquids, Glasses and Other Adventures in Thermodynamics and Statistical Mechanics, Celebrating Pablo Debenedetti 70th birthday
Type of participation: Participatory - invited/keynote talk
City of event: Princeton, United States of America
Date of event: 15/06/2023
End date: 18/12/2023
- 9** **Title of the work:** The Madrid force field for electrolytes in water and some thoughts on our understanding of the dielectric constant in computer simulations
Name of the conference: EMLG2022
Type of participation: Participatory - invited/keynote talk
City of event: Barcelona, Spain
Date of event: 12/09/2022
End date: 16/09/2022
- 10** **Title of the work:** The interfacial free energy of curved interfaces: some thoughts on classical nucleation theory
Name of the conference: Cecam workshop Current Challenges in Materials for Thermal Energy Storage
Type of participation: Participatory - invited/keynote talk
City of event: Zaragoza, Spain
Date of event: 08/06/2022
End date: 10/06/2022



- 11** **Title of the work:** Simulations of supercooled electrolyte solutions
Name of the conference: From water to colloidal water
Type of participation: Participatory - oral communication
City of event: Roma, Italy
Date of event: 06/06/2022
End date: 08/06/2022
- 12** **Title of the work:** The Madrid-2019 force field for electrolytes in water: An extension to the ions F⁻, Br⁻, I⁻, Rb⁺ and Cs⁺
Name of the conference: Water X
Type of participation: Participatory - invited/keynote talk
City of event: La Madalena, Cerdeña, Italy
Date of event: 28/05/2022
End date: 02/06/2022
- 13** **Title of the work:** COMPUTER SIMULATIONS OF ELECTROLYTES: the Madrid force field
Name of the conference: Cecam Workshop: Ion adsorption and electrokinetic transport at interfaces
Type of participation: Participatory - invited/keynote talk
Date of event: 04/05/2022
End date: 06/05/2022
City organizing entity: Avignon, France
- 14** **Title of the work:** Simulación por ordenador de agua y de agua marina
Name of the conference: Termo 2020
Type of participation: Participatory - Plenary session
City of event: Lanzarote, Spain
Date of event: 13/09/2020
End date: 16/09/2020
Organising entity: Grupo especializado de Termodinamica de la RSEF
- 15** **Title of the work:** Computer simulation of water: challenges after fifty years
Name of the conference: Thermodynamics 2019
Type of participation: Participatory - Plenary session
City of event: Punta Umbria (Huelva), Spain
Date of event: 26/06/2019
City organizing entity: United Kingdom
- 16** **Title of the work:** The Phase Behavior of Supercooled Water as Described by the TIP4P/ICE Model
Name of the conference: Roma Tre Congress on Water under Extreme Conditions
Type of participation: Participatory - invited/keynote talk
City of event: Roma, Italy
Date of event: 12/06/2019
End date: 14/06/2019
Carlos Vega.
- 17** **Title of the work:** Homogeneous nucleation of ice from computer simulations
Name of the conference: PPEPPD 2019 Conference
Type of participation: Participatory - oral communication
City of event: Vancouver, Canada
Date of event: 12/05/2019



End date: 16/05/2019

Carlos Vega de las Heras.

- 18 Title of the work:** Homogeneous nucleation of ice
Name of the conference: CECAM Heterogeneous nucleation of ice: The Ultimate Challenge for Molecular Modelling
Type of participation: Participatory - invited/keynote talk
City of event: Lausanne, Switzerland
Date of event: 09/2018
Carlos Vega. "Homogeneous nucleation of ice".
- 19 Title of the work:** Salts in water. Solubility, models and nucleation
Name of the conference: TENTH LIBLICE CONFERENCE on the Statistical Mechanics of Liquids
City of event: Srní (Sumava National Park), Czech Republic
Date of event: 17/06/2018
End date: 22/06/2018
Carlos Vega de las Heras.
- 20 Title of the work:** Water
Name of the conference: Thermodynamics 2017
Type of participation: Participatory - Plenary session
City of event: Edimburgo, United Kingdom
Date of event: 04/09/2017
Organising entity: Royal Society of Chemistry
- 21 Title of the work:** Simulaciones de agua: 50 años
Name of the conference: Ciclo de Conferencias del Centro de Investigaciones en Química Sostenible
Type of participation: Participatory - Plenary session
Date of event: 30/01/2017
- 22 Title of the work:** The Future of Chemical Physics
Name of the conference: The Future of Chemical Physics Conference
Type of participation: Organizational - Scientific and organizing committee
City of event: Oxford, United Kingdom
Date of event: 31/08/2016
End date: 02/09/2016
Organising entity: Journal of Chemical Physics
- 23 Title of the work:** Three worked examples for developing force fields: water, hydrates and NaCl solutions
Name of the conference: PPEPPD2016
Type of participation: Participatory - invited/keynote talk
Corresponding author: Yes
City of event: Oporto, Portugal
Date of event: 23/05/2016
End date: 27/05/2016
C. Vega.
- 24 Title of the work:** Computer simulations of water
Type of event: Seminar
Type of participation: Participatory - others
City of event: Basilea, Switzerland
Reasons for participation: Upon invitation



Date of event: 20/04/2016

Organising entity: Universidad de Basilea , Physical Chemistry Seminars

25 Title of the work: The fluid-solid transition in simulation studies of water: thermodynamic and kinetic aspects

Name of the conference: Workshop on Water at the Interface between Biology, Chemistry

Type of participation: Participatory - Plenary session

City of event: Trieste, Italy

Date of event: 05/10/2015

End date: 09/10/2015

26 Title of the work: Simulations of water

Name of the conference: 34th International Conference on Solution Chemistry

Type of participation: Participatory - invited/keynote talk

City of event: Praga, Czech Republic

Date of event: 30/08/2015

End date: 03/09/2015

Organising entity: IUPAC

27 Title of the work: Modelling water in computer simulations

Name of the conference: Equifase 2015

Type of participation: Participatory - Plenary session

City of event: Alicante, Spain

Date of event: 29/06/2015

End date: 02/07/2015

C. Vega.

28 Title of the work: The nucleation of ice from the seeding technique

Name of the conference: Workshop: Water under extreme conditions

Type of participation: Participatory - invited/keynote talk

City of event: Roma, Italy

Date of event: 10/06/2015

End date: 12/06/2015

C. Vega.

29 Title of the work: Homogeneous ice nucleation for several water models using the seeding technique

Name of the conference: Workshop: Ice nucleation

Type of participation: Participatory - oral communication

City of event: Princeton, United States of America

Date of event: 23/04/2015

End date: 24/04/2015

C. Vega.

30 Title of the work: Water: What can we learn from computer simulations ?

Name of the conference: Dechema

Type of participation: Participatory - Plenary session

City of event: Frankfurt, Germany

Date of event: 23/03/2015

End date: 24/03/2015

C Vega.



- 31 Title of the work:** Freezing of Water from Computer Simulations, invited talk
Name of the conference: Water – the Most Anomalous Liquid, Workshop
City of event: Estocolmo, Sweden
Date of event: 15/10/2014
- 32 Title of the work:** Freezing of water from computer simulations : Thermodynamic and Kinetic aspects, talk.
Name of the conference: NINTH LIBLICE CONFERENCE on the Statistical Mechanics of Liquids
City of event: Czech Republic
Date of event: 16/06/2014
- 33 Title of the work:** Nucleation of ice in water , invited talk
Name of the conference: WaterEurope
City of event: Zaragoza, Spain
Date of event: 09/06/2014
- 34 Title of the work:** Studies of the Fluid-solid Equilibria of Ices using Gromacs: Free Energies and Direct Coexistence Simulations,invited talk
Name of the conference: Workshop , Cecam From atoms to clouds: bridging the gap between atomistic simulation, surface science, atmospheric observation and climate modelling
City of event: Zurich, Switzerland
Date of event: 22/04/2014
Organising entity: Cecam
- 35 Title of the work:** Computer simulations of the phase diagram of water
Name of the conference: PPEPPD
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - invited/keynote talk
City of event: Iguazu, Argentina
Date of event: 20/05/2013
Carlos Vega de las Heras.
- 36 Title of the work:** Computer simulations of the phase diagram of water
Name of the conference: Conferencia plenaria invitada por la Universidad de Wisconsin
Type of event: Seminar **Geographical area:** Non EU International
Type of participation: Participatory - invited/keynote talk
City of event: Madison, United States of America
Date of event: 04/05/2013
Carlos Vega de las Heras.
- 37 Title of the work:** Computer simulations of the phase diagram of water
Name of the conference: Conferencia plenaria invitada por el Imperial College London
Type of event: Seminar **Geographical area:** European Union
Type of participation: Participatory - invited/keynote talk
City of event: Londres, United Kingdom
Date of event: 08/03/2013
Carlos Vega de las Heras.
- 38 Title of the work:** Supercooled water: simulation and experiment
Name of the conference: 8th Liquid Matter Conference
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - oral communication



City of event: Viena, Austria

Date of event: 16/09/2011

Jose Luis Fernandez Abascal; Carlos Vega de las Heras; Miguel Angel Gonzalez Gonzalez.

- 39 Title of the work:** Properties of supercooled water as obtained from computer simulations of the TIP4P/2005 model
Name of the conference: Cecam workshop Models for Bulk, Confined Water and Aqueous Solutions Upon Supercooling: State of the Art and Future Perspectives in Understanding Water Anomalies by Computer Simulations
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - invited/keynote talk
City of event: LAUSANNE, Switzerland
Date of event: 01/07/2011
City organizing entity: Switzerland
Carlos Vega de las Heras.
- 40 Title of the work:** Crystallisation studies of water: modelling , crystal growth and nucleation
Name of the conference: Cecam workshopCrystallization: from colloids to pharmaceuticals
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - invited/keynote talk
City of event: Lausanne, Switzerland
Date of event: 11/07/2010
City organizing entity: Switzerland
Carlos Vega de las Heras.
- 41 Title of the work:** Describing water using simple models
Name of the conference: Conferencia plenaria invitada por la Universidad de Luxemburgo
Type of event: Seminar **Geographical area:** European Union
Type of participation: Participatory - invited/keynote talk
City of event: Luxemburgo, Luxembourg
Date of event: 25/06/2010
Carlos Vega de las Heras.
- 42 Title of the work:** Can we describe water using computer simulations?
Name of the conference: Conferencia plenaria invitada por la Universidad de Oxford
Type of event: Seminar **Geographical area:** European Union
Type of participation: Participatory - invited/keynote talk
City of event: Oxford, United Kingdom
Date of event: 21/05/2010
Carlos Vega de las Heras.
- 43 Title of the work:** Can gas hydrate structures be described using classical simulations?
Name of the conference: CECAM Workshop. Molecular Simulation of Clathrate Hydrates
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - invited/keynote talk
City of event: DUBLIN, Ireland
Date of event: 06/05/2010
City organizing entity: Ireland
MARIA MARTIN CONDE; CARLOS VEGA DE LAS HERAS.



- 44** **Title of the work:** Can we describe water using computer simulations?
Name of the conference: Conferencia plenaria invitada por la Universidad La Sapienza
Type of event: Seminar **Geographical area:** European Union
Type of participation: Participatory - invited/keynote talk
City of event: Roma, Italy
Date of event: 28/01/2010
Carlos Vega de las Heras.
- 45** **Title of the work:** Five years simulating the phase diagram of water. What we learn something?
Name of the conference: International Conference Thermodynamics
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: LONDRES, United Kingdom
Date of event: 23/09/2009
City organizing entity: United Kingdom
JUAN LUIS ARAGONES GOMEZ; JOSE LUIS FERNANDEZ ABASCAL; LUIS GONZALEZ MAC-DOWELL;
EVA GONZALEZ NOYA; MARIA MARTIN CONDE; CARL MCBRIDE; CARLOS VEGA DE LAS HERAS.
- 46** **Title of the work:** The thickness of a liquid layer on the free surface of ice as obtained from computer simulation
Name of the conference: International Conference Thermodynamics
Type of event: Conference **Geographical area:** Non EU International
Type of participation: 'Participatory - poster
City of event: LONDRES, United Kingdom
Date of event: 23/09/2009
City organizing entity: United Kingdom
MARIA MARTIN CONDE; ANDREJ PATRYKIEJEV; CARLOS VEGA DE LAS HERAS.
- 47** **Title of the work:** The thickness of a liquid layer on the free surface of ice as obtained from computer simulation
Name of the conference: International Conference Thermodynamics
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: LONDRES, United Kingdom
Date of event: 23/09/2009
City organizing entity: United Kingdom
MARIA MARTIN CONDE; ANDREJ PATRYKIEJEV; CARLOS VEGA DE LAS HERAS.
- 48** **Title of the work:** Cinco años simulando el diagrama de fases del agua. Qué hemos aprendido ?
Name of the conference: Fisica Estadística 2009
Type of event: Conference **Geographical area:** National
Type of participation: Participatory - oral communication
Date of event: 10/09/2009
City organizing entity: HUELVA, Spain
JUAN LUIS ARAGONES GOMEZ; JOSE LUIS FERNANDEZ ABASCAL; LUIS GONZALEZ MAC-DOWELL;
EVA GONZALEZ NOYA; MARIA MARTIN CONDE; CARL MCBRIDE; CARLOS VEGA DE LAS HERAS.
- 49** **Title of the work:** Estudio por simulación del espesor de la capa líquida para la superficie libre del hielo
Name of the conference: Fisica Estadística 2009
Type of event: Conference **Geographical area:** National
Type of participation: 'Participatory - poster



Date of event: 10/09/2009

City organizing entity: HUELVA, Spain

MARIA MARTIN CONDE; ANDREJ PATRYKIEJEV; CARLOS VEGA DE LAS HERAS.

- 50** **Title of the work:** Diagrama de fases del agua por simulación computacional en la región de altas presiones: aparición de una fase de cristal plástico
Name of the conference: IV Escuela de Altas Presiones (MALTA-CONSOLIDER)
Type of event: Curso **Geographical area:** National
Type of participation: Participatory - oral communication
Date of event: 29/06/2009
City organizing entity: SANTANDER, Spain
JUAN LUIS ARAGONES GOMEZ; EVA GONZALEZ NOYA; MARIA MARTIN CONDE; CARLOS VEGA DE LAS HERAS.
- 51** **Title of the work:** The Dielectric constant of Ice
Name of the conference: 17th Symposium on Thermophysical Properties
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Boulder, United States of America
Date of event: 21/06/2009
City organizing entity: United States of America
LUIS GONZALEZ MAC-DOWELL; CARLOS VEGA DE LAS HERAS.
- 52** **Title of the work:** What ice can teach us about water interactions: a critical comparison of the performance of different water models
Name of the conference: Workshop, Molecular Simulations: Algorithms, Analysis, and Applications
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - poster
City of event: MINNEAPOLIS, United States of America
Date of event: 18/05/2009
City organizing entity: United States of America
JUAN LUIS ARAGONES GOMEZ; JOSE LUIS FERNANDEZ ABASCAL; MARIA MARTIN CONDE; CARLOS VEGA DE LAS HERAS.
- 53** **Title of the work:** A Successful Model for the Condensed Phases of Water : TIP4P/2005
Name of the conference: AiCHE meeting
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: PHILADELPHIA, United States of America
Date of event: 20/11/2008
City organizing entity: United States of America
JUAN LUIS ARAGONES GOMEZ; JOSE LUIS FERNANDEZ ABASCAL; MARIA MARTIN CONDE; CARLOS VEGA DE LAS HERAS.
- 54** **Title of the work:** What ice can teach us about water interactions: a critical comparison of the performance of different water models
Name of the conference: Faraday Discussion , 141
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - invited/keynote talk
City of event: EDIMBURGO, United Kingdom
Date of event: 27/08/2008



City organizing entity: United Kingdom

JUAN LUIS ARAGONES GOMEZ; JOSE LUIS FERNANDEZ ABASCAL; MARIA MARTIN CONDE;
CARLOS VEGA DE LAS HERAS.

- 55 Title of the work:** Absence of superheating for ice Ih with a free surface a new method of determining the melting point of different water models

Name of the conference: CCP5 (Collaborative Computational Project 5 - The Computer Simulation of Condensed Phase) Summer School

Type of event: Curso

Geographical area: European Union

Type of participation: 'Participatory - poster

City of event: SHEFFIELD, United Kingdom

Date of event: 06/07/2008

City organizing entity: United Kingdom

MARIA MARTIN CONDE; ANDREJ PATRYKIEJEV; CARLOS VEGA DE LAS HERAS.

- 56 Title of the work:** Properties of ices at 0K A test of water models

Name of the conference: CCP5 (Collaborative Computational Project 5 - The Computer Simulation of Condensed Phase) Summer School

Type of event: Curso

Geographical area: European Union

Type of participation: Participatory - oral communication

City of event: SHEFFIELD, United Kingdom

Date of event: 06/07/2008

City organizing entity: United Kingdom

JUAN LUIS ARAGONES GOMEZ; JOSE LUIS FERNANDEZ ABASCAL; EVA GONZALEZ NOYA; MARIA MARTIN CONDE; CARLOS VEGA DE LAS HERAS.

- 57 Title of the work:** Absence of superheating for ice Ih with a free surface a new method of determining the melting point of different water models

Name of the conference: SimBioMa (Conference on Molecular Simulations in Biosystems and Material Science)

Type of event: Conference

Geographical area: European Union

Type of participation: 'Participatory - poster

City of event: KONSTANZ, Germany

Date of event: 02/04/2008

City organizing entity: Germany

MARIA MARTIN CONDE; ANDREJ PATRYKIEJEV; CARLOS VEGA DE LAS HERAS.

- 58 Title of the work:** Determination of the phase diagram via computer simulation: methodology and application to water

Name of the conference: SimBioMa (Conference on Molecular Simulations in Biosystems and Material Science)

Type of event: Conference

Geographical area: European Union

Type of participation: 'Participatory - poster

City of event: KONSTANZ, Germany

Date of event: 02/04/2008

City organizing entity: Germany

JUAN LUIS ARAGONES GOMEZ; JOSE LUIS FERNANDEZ ABASCAL; LUIS GONZALEZ MAC-DOWELL; EVA GONZALEZ NOYA; MARIA MARTIN CONDE; EDUARDO SANZ; CARLOS VEGA DE LAS HERAS.

- 59 Title of the work:** Equation of state, thermal expansion coefficient and isothermal compressibility for ices Ih and II as obtained from computer simulation

Name of the conference: International Conference Thermodynamics



Type of event: Conference

Geographical area: Non EU International

Type of participation: 'Participatory - poster

City of event: PARIS, France

Date of event: 26/09/2007

City organizing entity: France

JUAN LUIS ARAGONES GOMEZ; EVA GONZALEZ NOYA; MARIA MARTIN CONDE; CARLOS MENDUIÑA FERNANDEZ; CARLOS VEGA DE LAS HERAS.

- 60 Title of the work:** Hydrate formation and salting out: New intermolecular potential models for methane in water and aqueous solutions

Name of the conference: International Conference Thermodynamics

Type of event: Conference

Geographical area: Non EU International

Type of participation: Participatory - oral communication

City of event: PARIS, France

Date of event: 26/09/2007

City organizing entity: France

HUGH DOCHERTY; AMPARO GALINDO; MARIA MARTIN CONDE; EDUARDO SANZ; CARLOS VEGA DE LAS HERAS.

- 61 Title of the work:** Phase diagram of an octahedral anisotropic patchy model potential

Name of the conference: Thermodynamics 2007

Type of event: Conference

Geographical area: European Union

Type of participation: Participatory - oral communication

Date of event: 26/09/2007

City organizing entity: Paris, France

J. P. K. Doye; A. A. Louis.

- 62 Title of the work:** Analysing the performance of water models to describe the phase diagram of water

Name of the conference: CECAM Workshop Modelling the structures and reactivity of silica and water: from molecule to macroscale

Type of event: Conference

Geographical area: Non EU International

Type of participation: Participatory - invited/keynote talk

City of event: LYON, France

Date of event: 17/09/2007

City organizing entity: France

JUAN LUIS ARAGONES GOMEZ; JOSE LUIS FERNANDEZ ABASCAL; LUIS GONZALEZ MAC-DOWELL; EVA GONZALEZ NOYA; MARIA MARTIN CONDE; EDUARDO SANZ; CARLOS VEGA DE LAS HERAS.

- 63 Title of the work:** New potential models and theoretical approaches for aqueous systems with salts and methane: hydrate formation and salting out

Name of the conference: Eleventh International Conference on Properties and Phase Equilibria for Product and Process Design

Type of event: Conference

Geographical area: Non EU International

Type of participation: 'Participatory - poster

City of event: CRETA, Greece

Date of event: 20/05/2007

City organizing entity: Greece

HUGH DOCHERTY; AMPARO GALINDO; MARIA MARTIN CONDE; EDUARDO SANZ; CARLOS VEGA DE LAS HERAS.

- 64** **Title of the work:** Ice: A fruitful source of information about liquid water
Name of the conference: EMLG/JMLG Annual Meeting, Liquids systems under extreme conditions
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - oral communication
City of event: Barcelona, Spain
Date of event: 22/09/2006
Jose Luis Fernandez Abascal; Ramon Garcia Fernandez; Luis Gonzalez MacDowell; Eduardo Sanz; Carlos Vega de las Heras.
- 65** **Title of the work:** Computer simulation studies of the phase diagram of water
Name of the conference: CCP5 Annual meeting
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - invited/keynote talk
City of event: BRADFORD, United Kingdom
Date of event: 04/09/2006
City organizing entity: United Kingdom
JOSE LUIS FERNANDEZ ABASCAL; RAMON GARCIA; LUIS GONZALEZ MAC-DOWELL; MARIA MARTIN CONDE; CARL MCBRIDE; EDUARDO SANZ; CARLOS VEGA DE LAS HERAS.
- 66** **Title of the work:** A comparison of the statistical associating fluid theory for potentials of variable range to Monte Carlo simulations for electrolyte solutions
Name of the conference: FOMMS (Foundations of Molecular Modeling and Simulation)
Type of event: Conference **Geographical area:** Non EU International
Type of participation: 'Participatory - poster
City of event: WASHINGTON, United States of America
Date of event: 09/07/2006
City organizing entity: United States of America
HUGH DOCHERTY; AMPARO GALINDO; MARIA MARTIN CONDE; EDUARDO SANZ; CARLOS VEGA DE LAS HERAS.
- 67** **Title of the work:** The phase diagram of water from computer simulation
Name of the conference: CECAM workshop. Patchy colloids, Proteins and Network forming liquids: Analogies and new insights from computer simulation
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: LYON, France
Date of event: 23/06/2006
City organizing entity: France
JOSE LUIS FERNANDEZ ABASCAL; LUIS GONZALEZ MAC-DOWELL; MARIA MARTIN CONDE; CARL MCBRIDE; EDUARDO SANZ; CARLOS VEGA DE LAS HERAS.
- 68** **Title of the work:** The phase diagram of water by computer simulation
Name of the conference: 7th Liblice Conference on the Statistical Mechanics of Liquids
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - oral communication
City of event: Lednice, Czech Republic
Date of event: 18/06/2006
Carlos Vega de las Heras.



- 69** **Title of the work:** What we have learn after three years of simulations of water and ices
Name of the conference: Thermodynamics 2005 (Royal Society of Chemistry)
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - oral communication
City of event: Sesimbra, Portugal
Date of event: 04/09/2005
Carlos Vega; Eduardo Sanz; Carl McBride; Jose Luis Fernandez Abascal; Luis Gonzalez MacDowell.
- 70** **Title of the work:** Determination of the phase diagram of water from computer simulation
Name of the conference: 6th Liquid Matter Conference (European Physical Society)
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - oral communication
City of event: Utrecht, United Kingdom
Date of event: 24/07/2005
Carlos Vega de las Heras; Eduardo Sanz; Carl McBride; Jose Luis Fernandez Abascal; Luis Gonzalez MacDowell.
- 71** **Title of the work:** Computer simulation of the phase diagram of water
Name of the conference: Statphys 22
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - invited/keynote talk
City of event: Bangalore, India
Date of event: 05/07/2004
Jose Luis Fernandez Abascal; Eduardo Sanz; Luis Gonzalez MacDowell; Carlos Vega de las Heras.
- 72** **Title of the work:** The phase diagram of the restricted primitive model
Name of the conference: Thermodynamics 2003 (Royal Society of Chemistry)
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - invited/keynote talk
City of event: Cambridge, United Kingdom
Date of event: 15/04/2003
Carlos Vega de las Heras.
- 73** **Title of the work:** Computer simulations of complex fluids
Name of the conference: 17th IUPAC Conference on Chemical Thermodynamics
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - invited/keynote talk
City of event: Rostock, Germany
Date of event: 04/08/2002
Carlos Vega de las Heras.
- 74** **Title of the work:** Simple models, complex fluids
Name of the conference: Global Phase Diagrams, International Bunsen Conference
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - invited/keynote talk
City of event: Colonia, Germany
Date of event: 16/08/2001
Carlos Vega de las Heras.



- 75** **Title of the work:** Understanding the phase diagram of quadrupolar fluids
Name of the conference: XXVI Statistical Mechanics Meeting
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - invited/keynote talk
City of event: Cuernavaca, Mexico
Date of event: 27/04/1997
Carlos Vega; Benito Garzon; Santiago Lago; Peter A. Monson.
- 76** **Title of the work:** The vapour-liquid equilibrium of n-alkanes
Name of the conference: 3rd European Liquid Matter Conference
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - oral communication
City of event: Norwich, United Kingdom
Date of event: 30/09/1996
Carlos Vega de las Heras; Benito Garzon; Luis Gonzalez MacDowell; Santiago Lago; Sofia Calero.
- 77** **Title of the work:** Equilibrio liquido-solido de sistemas moleculares e ionicos
Name of the conference: Fises. Fisica Estadistica
Type of event: Conference **Geographical area:** National
Type of participation: Participatory - oral communication
City of event: Zaragoza, Spain
Date of event: 21/09/1996
Carlos Vega de las Heras; Peter A. Monson.
- 78** **Title of the work:** Solid-fluid equilibria in systems of hard diatomics
Name of the conference: American Institute of Chemical Engineering Annual Meeting
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Miami, United States of America
Date of event: 11/05/1992
Carlos Vega de las Heras; P. A. Paras; Peter A. Monson.
- 79** **Title of the work:** Recent progress in understanding liquids
Name of the conference: Club de profesores de la Universidad de Harvad
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - invited/keynote talk
City of event: Boston, United States of America
Date of event: 05/03/1992
Carlos Vega de las Heras.
- 80** **Title of the work:** Monte Carlo study of rod like Kihara molecules
Name of the conference: NATO ASI
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - oral communication
City of event: Bath, United Kingdom
Date of event: 14/09/1988
Carlos Vega de las Heras; Daan Frenkel.

Other achievements

Stays in public or private R&D centres

- 1** **Entity:** Universidad de Lublin
City of entity: Poland
Start-End date: 01/07/2006 - 01/09/2006 **Duration:** 2 months - 2 days
Goals of the stay: Guest
Provable tasks: Estancia sabática en la Universidad de Lublin, POLONIA
- 2** **Entity:** University of Massachusetts
City of entity: United States of America
Start-End date: 01/07/1997 - 01/09/1997 **Duration:** 2 months - 2 days
Goals of the stay: Guest
Provable tasks: Estancia contrato NATO en USA para trabajar con el Prof. Peter A. Monson
- 3** **Entity:** University of Massachusetts
City of entity: United States of America
Start-End date: 01/09/1991 - 01/01/1993 **Duration:** 1 year - 4 months
Goals of the stay: Post-doctoral
Provable tasks: Estancia postdoctoral como becario Fulbright en USA bajo la supervisión del Profesor Peter A. Monson
- 4** **Entity:** Universidad de Cornell
City of entity: ITHACA, United States of America
Start-End date: 01/09/1990 - 01/11/1990 **Duration:** 2 months
Goals of the stay: Doctorate
Provable tasks: Estancia breve en UNIVERSIDAD DE CORNELL, ESTADOS UNIDOS DE AMERICA con cargo a mi beca de FPU y bajo la supervisión del Profesor Keith Gubbins
- 5** **Entity:** Universidad de Bochum (Alemania)
City of entity: (Ninguno), Germany
Start-End date: 14/04/1989 - 14/07/1989 **Duration:** 3 months
Goals of the stay: Doctorate
Provable tasks: Estancia breve en UNIVERSIDAD BOCHUN, ALEMANIA under supervision of Prof. Johann Fischer
- 6** **Entity:** FOM Institute for Atomic and Molecular Physics
City of entity: Holland
Start-End date: 01/09/1987 - 01/01/1988 **Duration:** 4 months
Goals of the stay: Doctorate
Provable tasks: Estancia breve en el Instituto de Física Atomica y Molecular para trabajar bajo la supervisión del Prof. Daan Frenkel

Periods of research activity and knowledge transfer

- 1** **Name of the action:** Sexenio CNEAI
Date of recognition: 20/06/2024
Type of activity: Research
Starting year: 2018
Completion date: 2023
Periodo cubierto: 2018, 2019, 2020, 2021, 2022, 2023/:/:2018, 2019, 2020, 2021, 2022, 2023
- 2** **Name of the action:** Sexenio CNEAI
Date of recognition: 12/06/2018
Type of activity: Research
Periodo cubierto: :/:/:
- 3** **Name of the action:** Sexenio CNEAI
Date of recognition: 20/06/2012
Periodo cubierto: :/:/:
- 4** **Name of the action:** Sexenio CNEAI
Date of recognition: 06/06/2006
Periodo cubierto: :/:/:
- 5** **Name of the action:** Sexenio CNEAI
Date of recognition: 30/06/2000
Periodo cubierto: :/:/:
- 6** **Name of the action:** Sexenio CNEAI
Date of recognition: 30/06/1998
Periodo cubierto: :/:/:

Summary of other achievements

- 1** **Description of the achievement:** H index =63 , 258 papers , 18300 citations
Accrediting entity: Web of Knowledge
Conferral date: 24/02/2025
- 2** **Description of the achievement:** Member of the evaluating committee of 38 PhD candidates
Conferral date: 24/02/2025
- 3** **Description of the achievement:** 38 papers with more than 100 citations
Accrediting entity: Weg of Science
Conferral date: 24/02/2025
- 4** **Description of the achievement:** Perteneciente a las lista de los mejores investigadores españoles de todas las areas de conocimiento.
Conferral date: 24/02/2025



- 5 Description of the achievement:** Seis tramos investigadores concedidos
Conferral date: 17/02/2025
- 6 Description of the achievement:** Seis tramos docentes concedidos (quinquenios)
Conferral date: 20/09/2021
- 7 Description of the achievement:** Cinco tramos de investigación (sexenios) concedidos
Conferral date: 01/10/2019
- 8 Description of the achievement:** Molecular Physics Lecture prize (In recognition of an outstanding contributions to the field)
Accrediting entity: Thermodynamics Conference Series
Conferral date: 05/09/2017
- 9 Description of the achievement:** Científico seleccionado para la presentación de nominaciones al Premio Nobel de Química (años 2013 y 2017)
Conferral date: 25/02/2017
- 10 Description of the achievement:** Para una búsqueda actualizada de citas utilizar mi Research ID en el Web of Science: C-5455-2009 (teclear esto como Author Identifier)
Conferral date: 19/11/2013
- 11 Description of the achievement:** Puesto 4009 en el ranking mundial de investigadores en Química más citados del ISI Web of Science (Essential Science Indicators)
Conferral date: 18/11/2013
- 12 Description of the achievement:** Reviewer (10-15 papers a year) for : Journal of Chemical Physics, J. Phys. Chem. B, J.Phys.Chem. A, J. Am. Chem. Soc., Nature, Molecular Physics, J.Phys.Condens.Matter, Ind.Engineering Chemistry Research, Physical Review E, Phys.Rev.Lett. , Fluid Phase Equilibria, J.Mol.Liq., J.Chem.Theo.Comput.
Conferral date: 14/12/2010
- 13 Description of the achievement:** Prize for PhD in Chemistry (1992) - Premio Extraordinario de Doctorado
Conferral date: 05/05/1992
- 14 Description of the achievement:** Post-doctoral Fulbright Fellow
Conferral date: 17/04/1991
- 15 Description of the achievement:** First National Prize for Bachelor in Chemistry (1987) -Primer premio Nacional de Licenciatura en Química
Conferral date: 06/06/1988
- 16 Description of the achievement:** First Prize for Bachelor in Chemistry at Complutense University (1987)-Premio Extraordinario de Licenciatura
Conferral date: 05/05/1988