

Currículum vitae

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Publication list

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1. AUTHORS :S.Lago y C.Vega
Title: *A generalization for mixtures of a fast algorithm to calculate some orientational averages*
Journal: *Computers and Chemistry* **12**, 343–356, (1988).

 2. AUTHORS : C.Vega y D.Frenkel
Title: *Monte Carlo study of rod like molecules. A test of perturbation theory for the Kihara model*
Journal: *Molecular Physics* **67**, 633–650, (1989).

 3. AUTHORS :C.Vega,B.Saager y J.Fischer
Title: *Molecular dynamics studies for the new refrigerant R152a with simple model potentials*
Journal:*Molec.Phys.*, **68**, 1079-1093, (1989).

 4. AUTHORS : T.Boublik, C.Vega y M.D.Peña
Title: *Equation of state of chain molecules*
Journal: *J.Chem.Phys.* **93**, 730–736 (1990).

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 6. AUTHORS : C.Vega y S.Lago
Title: *Molecular dynamics study of propane using two simple potential models*
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Title: *Perturbation theory of angular Kihara fluids*
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 9. AUTHORS : P.Sevilla, S.Lago, C.Vega y P.Padilla
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Title: *Improved perturbation theory of Kihara fluids*
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13. AUTHORS : C.Vega
Title: *Perturbation theory of hard quadupolar fluids*
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14. AUTHORS : C.Vega y K.E.Gubbins
Title: *Monte Carlo study of quadrupolar Kihara fluids*
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15. AUTHORS : C.Vega, S.Lago y P.Padilla Title: *Thermodynamic properties of molecular fluids of any geometry from perturbation theory* Journal: J.Phys.Chem. **96**, 1900–1905, (1992).

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17. AUTHORS : C.Vega, E.P.A.Paras y P.A.Monson Title: *Solid-fluid equilibria for hard dumbbells via Monte Carlo simulation* Journal: J.Chem.Phys. **96**, 9060–9072, (1992).

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CLAVE: A
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118. AUTHORS : C.Vega and E.G.Noya TITLE: *Revisiting the Frenkel-Ladd method to compute the free energy of solids: the Einstein molecule approach* JOURNAL: J.Chem.Phys. , **127**, 154113 , (2007).
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119. AUTHORS : E.G.Noya, C.Menduiña, J.L.Aragones y C.Vega TITLE: *Equation of state, thermal expansion coefficient and isothermal compressibility for ices I_h, II, III, V and VI, as obtained from computer simulation* JOURNAL: J.Phys.Chem.B , **111**, 15877-15888, (2007).
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120. AUTHORS : J.L.F.Abascal y C.Vega TITLE: *The water forcefield: importance of dipolar and quadrupolar interactions* JOURNAL: J.Phys.Chem.C , **111**, 15811-15822, (2007).
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121. AUTHORS : J.L.F. Abascal, R. García Fernández, L.G. MacDowell, E. Sanz and C. Vega TITLE: *Ice: a fruitful source of information about liquid water* JOURNAL: J.Mol.Liq. , **136**, 214-220, (2007).
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122. AUTHORS : J.B.Caballero, E.G.Noya y C.Vega TITLE: *Complete phase behaviour of the symmetrical colloidal electrolyte* JOURNAL: J.Chem.Phys. , **127**, 244910-1-244910-7, (2007).
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123. AUTHORS (p.o. de firma): C.Vega, E.Sanz, J.L.F.Abascal and E.G.Noya TITLE: *Determination of phase diagrams via computer simulation: methodology and applications to water, electrolytes and proteins* JOURNAL: J.Phys.Condens.Matter **20**, 153101, (2008).
-
124. AUTHORS (p.o. de firma): E.G.Noya , C.Vega y E.de Miguel TITLE: *Determination of the melting point of hard spheres from direct coexistence simulation methods* JOURNAL: J.Chem.Phys. **128**, 154507, (2008).
-
125. AUTHORS (p.o. de firma): M.M.Conde, C.Vega y A.Patrykiewicz TITLE: *The thickness of a liquid layer on the free surface of ice as obtained from computer simulation.* JOURNAL: J.Chem.Phys. **129**, 014702, (2008).
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126. AUTHORS (p.o. de firma): F. Gamez, S. Lago, B.Garzon, P.Merkling and C.Vega TITLE: *Vapor-liquid equilibrium of fluids composed by oblate molecules.* JOURNAL: Molecular Physics , **106**, 1331-1339, (2008).
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127. AUTHORS (p.o. de firma): E.G.Noya, M.M.Conde and C.Vega TITLE: *Computing the free energy of molecular solids by the Einstein molecule approach: Ices XIII and XIV and a simple model of proteins.* JOURNAL: J.Chem.Phys. , **129**, 104704-1, 104704-16, (2008).
-
128. AUTHORS (p.o. de firma): C.Vega, J.L.F.Abascal, M.M.Conde and J.L.Aragones TITLE: *What ice can teach us about water interactions : a critical comparison of the performance of different water models* JOURNAL: Faraday Discussions , **141**, 251-276, (2009).
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129. AUTHORS (p.o. de firma): J.L.Aragones, M.M. Conde , E.G.Noya and C.Vega TITLE: *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* JOURNAL: Phys.Chem.Chem.Phys. , **11**, 543-555, (2009).
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130. AUTHORS (p.o. de firma): J.L.F.Abascal, E.Sanz and C.Vega TITLE: *Triple points and coexistence properties of the dense phases of water calculated using computer simulation* JOURNAL: Phys.Chem.Chem.Phys. , **11**, 556-562, (2009).
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131. AUTORES (p.o. de firma): H.L.Pi, J.L.Aragones, C.Vega, E.G.Noya, J.L.Abascal , M.A.Gonzalez and C.McBride TÍTULO: *Anomalies in water as obtained from computer simulations of the TIP4P/2005 model: density maxima, and density, isothermal compressibility and heat capacity minima* REVISTA: Molec. Phys. , **107**, 365, (2009). CLAVE: A
-
132. AUTORES (p.o. de firma): J.L.Aragones y C.Vega TÍTULO: *Plastic crystal phases of simple water models* REVISTA: J.Chem.Phys. , **130**, 244504, (2009). CLAVE: A
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133. AUTORES (p.o. de firma): C.McBride,C.Vega,E.G.Noya,R.Ramirez and L.M.Sese TÍTULO: *Quantum contribution in the ice phases: the path to a newempirical model for water: TIP4PQ/2005* REVISTA: J.Chem.Phys. , 131, 024506 , (2009). CLAVE: A
-
134. AUTORES (p.o. de firma): M.M.Conde, C. Vega, G.A.Tribello and B.Slater TÍTULO: *The phase diagram of water at negative pressures: Virtual ices* REVISTA: J.Chem.Phys. , 131, 034510 , (2009). CLAVE: A
-
135. AUTORES (p.o. de firma): E.G.Noya ,C.Vega, L.M.Sese y R.Ramirez TÍTULO: *Quantum effects on the maximum in density of water as described by the TIP4PQ/2005 model* REVISTA: J.Chem.Phys. , 131 124518 (2009) . CLAVE: A
-
136. AUTORES (p.o. de firma): C.Vega , M. M. Conde , C. McBride , J.L.F. Abascal , E.G. Noya , R.Ramirez y L.M.Sese TÍTULO: *Heat capacity of water: a signature of nuclear quantum effects* REVISTA: J.Chem.Phys. , 132, 046101 (2010) . CLAVE: A
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137. AUTORES (p.o. de firma): B. Gonzalez , E.G.Noya , C. Vega y L. M. Sese TÍTULO: *Nuclear Quantum Effects in Water Clusters: The Role of the Molecular Flexibility* REVISTA: J.Phys.Chem. B , 114, 2484-2492 (2010). CLAVE: A
-
138. AUTORES (p.o. de firma): D.G.Salgado y C. Vega TÍTULO: *Melting point and phase diagram of methanol as obtained from computer simulations of the OPLS model* REVISTA: J.Chem.Phys. , 132 , 094505 , (2010). CLAVE: A
-
139. AUTORES (p.o. de firma): M. M. Conde, C.Vega, C. McBride, E.G.Noya, R.Ramirez y L. M. Sese TÍTULO: *Can gas hydrate structures be described using classical simulations?* REVISTA: J.Chem.Phys. , 132, 114503 , (2010). CLAVE: A
-
140. AUTORES (p.o. de firma): L. G. MacDowell y C. Vega TÍTULO: *Dielectric Constant of Ice Ih and Ice V: A Computer Simulation Study* REVISTA: J. Phys. Chem. B, , 114, 6089, (2010). CLAVE: A
-

12. Conferences

1. AUTHORS: S.Lago, P.Padilla y C.Vega

Title: Gas-gas equilibria from a thermodynamical perturbation theory

CONGRESS : Internacional. 9th IUPAC Conference on Chemical Thermodynamic

Place : Lisboa, Portugal

DATE : Fecha: Julio 1986

2. AUTHORS: P.Padilla, C.Vega S.Lago y P.Sevilla

Title: A bridge between Fischer and Boublik thermodynamic perturbation theories

Contribution : Poster

CONGRESS : Internacional . 6th International Conference on Mixtures of non electrolites and Intermolecular Interactions

Place : Merseburg, Alemania

DATE : Agosto 1988

3. AUTHORS: P.Sevilla, S.Lago ,P.Padilla y C.Vega

Title: Numerical solution of the Percus-Yevick equation for hard and soft spherocylinders

Contribution : Invited Talk

CONGRESS : Internacional. 10th IUPAC Conference on Chemical Thermodynamics

Place : Praga, Checoslovaquia

DATE : Agosto 1988

4. AUTHORS: C.Vega y D.Frenkel

Title: Monte Carlo study of rod like Kihara molecules

Contribution : Talk

CONGRESS : Internacional. NATO ASI

PLACE: Bath, Reino Unido

DATE : Septiembre 1988

5. AUTHORS: P.Padilla, C.Vega, S.Lago, A.Alguacil, B.Garzón y P.Saiz

Title: Bridge perturbation theory applied to hidrocarbons: results for linear carbon skeleton and some hints for non-linear

Contribution : Poster

CONGRESS : Internacional. 4th International Conference on Thermodynamic of solution of non-electrolites

Place : Santiago de Compostela, España

DATE : Septiembre 1989

6. AUTHORS: C.Vega ,S.Lago y P.Padilla

Title: Propane and butane conformers: preliminary results from a perturbation theory

Contribution : Poster

CONGRESS : Internacional. 3th Liblice Conference on the Statistical Mechanics of Liquids

Place : Praga, Checoslovaquia

DATE : Mayo 1990

7. AUTHORS: S.Lago, C.Vega, P.Padilla y B.Garzón

Title: Vapor-liquid equilibrium of molecular liquids with different geometries from perturbation theory

Contribution : Poster

CONGRESS : Internacional. First Liquid Matter Conference of the European Physical Society

Place : Lyon, Francia

DATE : Julio 1990

8. AUTHORS: S.Lago ,C.Vega , B.Garzón , P.Padilla y J.L.Lopez Martin

Title: Conformational shift in liquid state and liquid-vapor equilibrium for n-butane from perturbation theory

Contribution : Poster

CONGRESS : Internacional. Faraday Symposium 27 on the conformations of flexible molecules in fluid phases

Place : Southampton, Reino Unido

DATE : Diciembre 1991

9. AUTHORS: C.Vega, S.Lago, E.de Miguel y L.F.Rull
Title: Liquid vapor equilibria of linear Kihara molecules
Contribution : Poster
CONGRESS : Internacional. 18th Statphys
Place :Berlin, Alemania
DATE : Agosto 1992

10. AUTHORS: C.Vega
Title: **Recent progress in understanding liquids**
Contribution : **Conferencia plenaria Invitada**
Place : **Club de profesores de la Universidad de Harvard, USA**
DATE : **Marzo 1992**

11. AUTHORS: C.VEGA, E.P.A.PARAS Y P.A.MONSON
Title: **SOLID-FLUID EQUILIBRIA IN SYSTEMS OF HARD DIATOMICS**
Contribution : **COMUNICACIÓN ORAL (30 MINUTOS)**
CONGRESS: *Internacional. American Institute of Chemical Engineering Annual Meeting*
Place : **MIAMI, FLORIDA, USA**
Date : **1992**

12. AUTHORS: A.Gil Villegas, F.del Rio y C.Vega
Title: Solution of the RHNC equation for the square well fluid
Contribution: Poster
CONGRESS : Nacional. XXXV congreso de la Sociedad Mexicana de Física
Place :Puebla, México
DATE : Octubre 1992

13. AUTHORS: J.L.L.Martin, B.Garzón, S.Lago, E.Lopez y C.Vega
Title: Algunos resultados de interés en Ingeniería Química con bases relativamente rigurosas de Mecánica Estadística
Contribution: Poster
CONGRESS : Nacional. Física Estadística 93
Place :El Escorial, Madrid
DATE : Mayo 1993

14. AUTHORS: B.Garzon, E.de Miguel, C.Vega, L.F.Rull y S.Lago
Title: Vapor-liquid equilibria of dipolar linear Kihara fluids
Contribution: Poster
CONGRESS : Internacional. Second liquid Matter Conference of the European Physical Society
Place : Florencia, Italia
DATE : Septiembre 1993

15. AUTHORS: C.Vega
Title: Vapor liquid equilibrium of dipolar linear Kihara fluids
Contribution: Poster
CONGRESS : Internacional. IV Liblice Conference on the Statistical Mechanics of Liquids
Place :Checoslovaquia
DATE : Junio 1994

16. AUTHORS: B.Garzon, C.Vega, S.Lago y L.F.Rull
Title: Simulación del equilibrio líquido vapor de fluidos lineales dipolares y cuadrupolares.
Contribution: Talk invitada
CONGRESS : Internacional. Equilibrio de Fases (EQUIFASE).
Place :Caracas, Venezuela
DATE : Junio 1995

17. AUTHORS: C.VEGA y P.A.MONSON
Title: **EQUILIBRIO LÍQUIDO-SÓLIDO DE SISTEMAS MOLECULARES E IÓNICOS**
Contribution: **COMUNICACIÓN ORAL (30 MINUTOS)**
CONGRESS: *Nacional. FÍSICA ESTADÍSTICA 96*

Place : ZARAGOZA
AÑO: 1996

18. AUTHORS: C.VEGA

Title: **THE FLUID-SOLID EQUILIBRIUM OF IONIC SYSTEMS**
Contribution: **COMUNICACIÓN ORAL (30 MINUTOS)**
CONGRESS: *Internacional. PRE-LIQUID MATTER CONFERENCE*
Place : **Universidad de Sheffield (REINO UNIDO)**
AÑO: 1996

19. AUTHORS: C.VEGA,B.GARZON,L.G.MACDOWELL,S.LAGO Y S.CALERO

Title: **THE VAPOUR-LIQUID EQUILIBRIUM OF N-ALKANES**
Contribution: **COMUNICACIÓN ORAL (30 MINUTOS)**
CONGRESS: *Internacional. THIRD EUROPEAN LIQUID MATTER CONFERENCE*
Place : **NORWICH (REINO UNIDO)**
DATE : 1996

20. AUTHORS: P.Padilla y C.Vega

Title: A computer simulation study of the similarities between a system of fluid alkanes and a mixture of alkanes and spherical particles
Contribution : Talk invitada
CONGRESS :*Internacional. 10th Nordic Symposium on Computer Simulation*
Place :Tallin, Estonia
DATE : Julio 1996

21. AUTHORS: C.VEGA,B.GARZON,S.LAGO AND P.MONSON

Title: **UNDERSTANDING THE PHASE DIAGRAM OF QUADRUPOLAR FLUIDS**
Contribution: **CONFERENCIA INVITADA (1 HORA)**
CONGRESS: *Internacional. XXVI STATISTICAL MECHANICS MEETING*
Place : **CUERNAVACA ,MEXICO.**
AÑO: 1997

22. AUTHORS: C.Vega, L.G.MacDowell y P.Padilla

Title: Coeficientes del virial y ecuación de estado de moléculas duras flexibles
Contribution: Poster
CONGRESS : *Nacional. Física Estadística 97*
Place : Getafe, España
DATE : Septiembre 1997

23. AUTHORS:L.G.MacDowell, C.Vega

Title: Vapor-Liquid equilibrium of linear and branched alkanes from a mean field perturbation theory
Contribution: Poster
CONGRESS : *Nacional. Primera reunión nacional sobre Estado Líquido*
Place : Aguadulce, Almería
DATE : Julio 1998

24. AUTHORS: L.G.MacDowell y C.Vega

Title: Vapor-Liquid equilibrium of linear and branched alkanes
Contribution: Poster
CONGRESS : *Internacional. European Molecular Liquids Conference*
PLACE: Mureau, Austria
DATE : Noviembre 1998

25. AUTHORS: L.G.MacDowell, A.L.Rodriguez and C.Vega

Title: Phase coexistence and critical behavior of linear and branched alkanes mixtures from perturbation theory
Contribution:Poster
CONGRESS : *Internacional. Thermodynamics 99*
PLACE: Londres, Reino Unido
DATE : Marzo 1999

26. AUTHORS: C.Vega, J.M.Labaig, L.G.MacDowell
Title: Second, Third and fourth virial coefficients of polymers: a Monte Carlo study
Contribution: Poster
CONGRESS : Internacional. IV Liquid Matter Conference of the European Physical Society PLACE:Granada, España
DATE : Julio 1999

27. AUTHORS: C.Vega y P.A.Monson
Title: Fluid-Solid equilibrium of molecular systems via computer simulation
Contribution: Poster
CONGRESS : Internacional. European Research Conference: Solid-Fluid Interfaces 1999
PLACE:Castelvechio Pascoli, Italia
DATE : Septiembre 1999

28. AUTHORS:C.Vega
Title: Aplicaciones de la Mecánica Estadística al estudio de hidrocarburos
Contribution: Talk invitada
CONGRESS : Primer ciclo de conferencias de Física Básica y Aplicada de la Universidad de Huelva
PLACE:Huelva, España
DATE : Mayo 2000

29. AUTHORS:C.McBride, L.G.MacDowell y C.Vega
Title: The liquid crystal phase: a study of flexibility using a hard model
Contribution: Poster
CONGRESS :Nacional. Fises 2000
PLACE: Santiago de Compostela, España
DATE : Septiembre 2000

30. AUTHORS: C.Mendiña, C.McBride y C.Vega
Title: Second virial coefficient calculations of quadrupolar linear molecules and their mixtures
Contribution: Poster
CONGRESS : Internacional. 16th IUPAC Conference on Chemical Thermodynamics
PLACE:Halifax, Canada
DATE : Agosto 2000

31. AUTHORS: L.G.MacDowell, M.Muller, P.Virnau, C.Vega y K.Binder
Title: Critical behavior of chain molecules and their mixtures and prediction of the critical point of polyethylene
Contribution: Comunicación oral
CONGRESS : Internacional. Thermodynamics 2001
PLACE:Bristol, Reino Unido.
DATE : Abril 2001.

32. AUTHORS: C.Vega
Title: **The effect of flexibility on the phase diagram of simple molecular models.**
Contribution: **Conferencia invitada (1 hora)**
CONGRESS : **Seminarios del Dep.Qímica de la U.Durham.**
PLACE: **Universidad of Durham, Reino Unido.**
DATE : **Mayo 2001.**

33. AUTHORS:C.Vega
Title: **Simple models, complex fluids**
Contribution: **Conferencia plenaria invitada (1 hora)**
CONGRESS : **Internacional. Global Phase Diagrams, International Bunsen Conference**
PLACE:**Colonia, Alemania**
DATE : **Agosto 2001**

34. AUTHORS: C.Vega
Title: **Computer simulations of complex fluids**
Contribution: **Talk invitada**

CONGRESS : **Internacional. 17th IUPAC Conference on Chemical Thermodynamics**
PLACE: **Rostock, Alemania**
DATE : **Agosto 2002**

35. AUTHORS: C.Vega

Title: **The phase diagram of the restricted primitive model**

Contribution: **Talk invitada**

CONGRESS : **Internacional. Thermodynamics 2003 (Royal Society of Chemistry)**

PLACE: **Cambridge, United Kingdom.**

DATE : **Abril, 2003.**

36. AUTHORS: C.Vega, F.J.Blas and A.Galindo

Title: **Extension of the Thermodynamic Perturbation Theory of Wetheim to Model Solid Phases of Attractive Chain Molecules**

Contribution: **Talk**

CONGRESS : **Internacional. 15th SYMPOSIUM ON THERMOPHYSICAL PROPERTIES**

PLACE: **Boulder, Colorado, USA.**

DATE : **Junio , 2003.**

37. AUTHORS: L.G.MacDowell, C.McBride, C.Menduiña, E.Sanz y C.Vega

Title: **Simulación por ordenador de fluidos moleculares**

Contribution: **Talk**

CONGRESS : **Nacional. Primera reunión de expertos en fluidos comprimidos**

PLACE: **Madrid, Campo de las Naciones.**

DATE : **12-14 Noviembre 2003.**

38. AUTHORS: L.G.MacDowell, C.Vega, P.Virmau, M.Muller and K.Binder

Title: **Polymer-solvent mixtures: a quantitative comparison between TIPT1 and computer simulation**

Contribution: **Poster**

CONGRESS : **Internacional. SAFT Simposium.**

PLACE: **Barcelona.**

DATE : **12 Diciembre 2003.**

39. AUTHORS: J.L.F.Abascal, E.Sanz, L.G.MacDowell and C.Vega

Title: **Computer simulation of the phase diagram of water**

Contribution: **Talk invitada**

CONGRESS : **Internacional. Statphys 22.**

PLACE: **Bangalore, India.**

DATE : **5-9 Julio 2004**

40. AUTHORS: E.Sanz, C.Vega, J.L.F.Abascal, L.G.MacDowell and C.McBride

Title: **Phase diagram, combinatorial entropy and metastability in water.**

Contribution: **Poster.**

CONGRESS : **Internacional. Conference on Disorder, complexity and Biology (DISCOMBO4).**

PLACE: **Varanasi, India.**

DATE : **12-15 Julio 2004**

41. AUTHORS: E.Sanz, C.Vega, J.L.F.Abascal and L.G.MacDowell

Title: **The phase diagram of water from computer simulation**

Contribution: **Poster**

CONGRESS : **Internacional. SIMU, bridging the scales.**

PLACE: **Genova, Italia.**

DATE : **29-31 Agosto 2004.**

42. AUTHORS: F. J. Blas, A. Galindo, C. Vega, E. Sanz, and E. de Miguel

Title: **Global phase behaviour of chain molecules: flexible and rigid models**

Contribution: **poster**

CONGRESS : **10th International Conference on Properties and Phase Equilibria for Product and Process Design, Snow-bird**

PLACE: **Utah, USA**

DATE : 16-21 May 2004

43. AUTHORS: J.L.F.Abascal, E.Sanz, C.Vega, C.McBride and L.G.MacDowell

Title: What we have learn after three years of simulations of water and ices

Contribution: Talk

CONGRESS : Thermodynamics 2005 (organizado por la Royal Society of Chemistry)

PLACE: Sesimbra, Portugal

44. AUTHORS: C.Vega, E.Sanz, C.McBride, J.L.F.Abascal and L.G.MacDowell

Title: Determination of the phase diagram of water from computer simulation

Contribution: Talk

CONGRESS : 6th Liquid Matter Conference (organizado por la European Physical Society) , Julio 2005

PLACE: Utrecht, Holanda

45. AUTHORS: C.Vega

Title: The phase diagram of water by computer simulation

Contribution: Talk

CONGRESS : 7th Liblice Conference on the Statistical Mechanics of Liquids, Junio 2006

PLACE: Lednice, Republica Checa

46. AUTHORS: C.Vega,E.Sanz,J.L.F.Abascal,L.G.MacDowell, C.McBride, R.Garcia and M.M.Conde

Title: The phase diagram of water from computer simulation

Contribution: Talk

CONGRESS : Cecam workshop. Patchy colloids, Proteins and Network forming liquids: Analogies and new insights from computer simulations , Junio 2006.

PLACE: Lyon, Francia

47. AUTHORS: H.Docherty, A.Galindo, M.M.Conde, E.Sanz y C.Vega

Title: A comparison of the statistical associating fluid theory for potentials of variable range to Monte Carlo simulations for electrolyte solutions

Contribution: Poster

CONGRESS : FOMMS (Foundations of Molecular Modeling and Simulation), Julio 2006

PLACE: Washington, Estados Unidos.

48. AUTHORS: J.L.F. Abascal, R. García Fernández, L.G. MacDowell, E. Sanz, C. Vega

Title: Ice: A fruitful source of information about liquid water

Contribution: Talk

CONGRESS : EMLG/JMLG Annual Meeting, Liquids systems under extreme conditions , Septiembre 2006

PLACE: Barcelona

49. AUTHORS: C.Vega,E.Sanz,J.L.F.Abascal,L.G.MacDowell, C.McBride, R.Garcia and M.M.Conde

Title: Computer simulation studies of the phase diagram of water

Contribution: Talk plenaria invitada.

CONGRESS : CCP5 Annual meeting, Septiembre del 2006.

PLACE: Bradford, Reino Unido

50. Authors: Amparo Galindo , Hugh Docherty, Eduardo Sanz, Carlos Vega y Maria M. Conde

Title: NEW POTENTIAL MODELS AND THEORETICAL APPROACHES FOR AQUEOUS SYSTEMS WITH SALTS AND METHANE: HYDRATE FORMATION AND SALTING OUT

Contribution: Poster.

CONGRESS : PPED (Properties and Phase Equilibria for Product and Process Design, Mayo 2007.

Place: Creta, Grecia.

51. Autores: C. Vega

Título: Water at interfaces interactions

Tipo de participación: Talk Invitada (

Congreso: Workshop on Theory and Computer Simulation of Inhomogeneous Fluids

Lugar de celebración: Madrid

Mes: Mayo

Año: 2007

52. Authors: Carlos Vega, J.L.F.Abascal,E.Sanz,L.G.MacDowell,E.G.Noya,M.M.Conde and J.L.Aragones
Title: Analysing the performance of water models to describe the phase diagram of water
Contribution: Talk.
CONGRESS : Cecam workshop Modelling the structures and reactivity of silica and water: from molecule to macroscale, Septiembre del 2007.
Place: Lyon, Francia.

53. Authors: E.G.Noya, C.Vega, J.P.K.Doye, A.A.Louis
Title: Phase diagram of an octahedral anisotropic patchy model potential
Contribution: Talk.
CONGRESS : Thermodynamics , Septiembre 2007.
Place: Paris, Francia.

54. Authors: H. Docherty , A. Galindo , E. Sanz, C. Vega, M. M. Conde
Title: Hydrate formation and salting out: new potential models for methane in water and aqueous solutions
Contribution: Talk.
CONGRESS : Thermodynamics , Septiembre 2007.
Place: Paris, Francia.

55. Authors: Poster 1. E.G.Noya, C.Vega, J.P.K.Doye, A.A.Louis Poster 2. C. Vega, E. Sanz, J. L. F. Abascal, L. G. MacDowell, E. G. Noya, M. M. Conde, J. L. Aragonés Poster 3. J.L. Aragonés, E.G. Noya, J.L.F. Abascal, C. Vega Poster 4. M.M. Conde , C. Vega , A. Patrykiewicz
Title: Poster 1. Determination of the phase diagram of a simple model of proteins via computer simulation Poster 2. Determination of the phase diagram via computer simulation: methodology and application to water Poster 3. Properties of ices at 0K A test of water models Poster 4. Absence of superheating for ice Ih with a free surface a new method of determining the melting point of different water models
Contribution: Posters.
CONGRESS : Simbioma, Abril , 2008.
Place: Konstanz, Alemania.

56. Authors: Gary N. I. CLARK, Amparo GALINDO, George JACKSON, Carlos VEGA
Title: The use of spectroscopic data for the degree of association to determine optimal models for water in theoretical and computer simulation methods.
Contribution: Poster.
CONGRESS : Liquid Matter Conference, Julio 2008.
Place: Lund, Suecia.

57. Authors: J.L. Aragonés, E.G. Noya, J.L.F. Abascal, M.M. Conde, C. Vega
Título: Properties of ices at 0K A test of water models
Tipo de participación: Talk
Congreso: CCP5 (Collaborative Computational Project 5 - The Computer Simulation of Condensed Phase)
Lugar de celebración: Sheffield (Reino Unido) **Mes:** Julio **Año:** 2008

58. Authors: C.Vega,J.L.F.Abascal,M.M.Conde and J.L.Aragones
Title: What ice can teach us about water interactions : a critical comparison of the performance of different water models
Contribution: Conferenciante invitado.
CONGRESS : Faraday Discussion , 141 , Agosto 2008.
Place: Edimburgo, Reino Unido

59. Authors: C.Vega,J.L.F.Abascal,M.M.Conde and J.L.Aragones
Title: A Successful Model for the Condensed Phases of Water : TIP4P/2005
Contribution: Talk.
CONGRESS : AiCHE meeting , Noviembre 2008.
Place: Philadelphia, USA.

60. Authors: C.Vega
Title: Simulation studies of water at the vapor-liquid, vapor-solid and liquid-solid interfaces.

Contribution: **Talk.**

CONGRESS : **Ice/Vapor Interface: Molecular Modeling and Experiments Ice workshop , Noviembre 2008.**

Place: **Praga, Republica Checa.**

61. Authors: C.Vega

Title: **Estudios mediante simulacion por ordenador del diagrama de fases del agua**

Contribution: **Conferencia invitada.**

CONGRESS : **Jornadas de Termodinamica, Orense Diciembre, 2009.**

Place: **Orense, Espana.**

THESIS SUPERVISED AND FINISHED SUCCESSFULLY

Title: TERMODINAMICA ESTADISTICA DE MOLECULAS FLEXIBLES: TEORIA Y SIMULACION

PhD Student : LUIS GONZÁLEZ MACDOWELL

University : Universidad Complutense

Faculty/School : Ciencias Químicas

Title: EQUILIBRIO TERMODINÁMICO DE SÓLIDOS MEDIANTE SIMULACIÓN MOLECULAR

Student : EDUARDO SANTIAGO SANZ GARCIA

University : Universidad Complutense

Faculty/School : Ciencias Químicas

Publications analysis.

Revista (impacto)	Número
Physical Review Letters(6)	3
Faraday Discussion (5)	1
Journal of Chemical Physics (3.3)	66
Journal of Physical Chemistry (4)	5
Journal of Physical Chemistry B (4)	5
Journal of Physical Chemistry C (4)	2
Physical Review E (2.1)	6
Chemical Physics Letters (2.3)	2
Molecular Physics (1.85)	31
Computer Physics Communications (1.51)	1
Physical Chemistry and Chemical Physics (2.5)	8
J.Phys.Condens.Matter(1.4)	3
Fluid Phase Equilibria(0.8)	1
Journal of Molecular Liquids (1.0)	3
Computers and Chemistry (0.8)	2
Physical Chemistry of Liquids (0.5)	1
TOTAL number of papers :	140

Citation analysis, updated , May 2010.

Total number of citations : 2869

Papers with more than 100 citations : 4

H (h-index) = 29

Algorithm search for ISI :

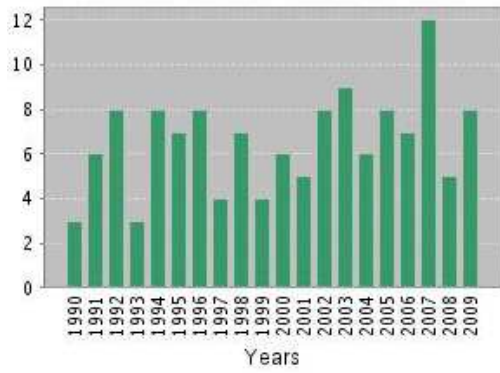
AUTHOR: VEGA C

ADDRESS: quim fis or fac ciencias QUIM and complutense or amherst or bochum or amsterdam

Research ID: <http://www.researcherid.com/rid/C-5455-2009>

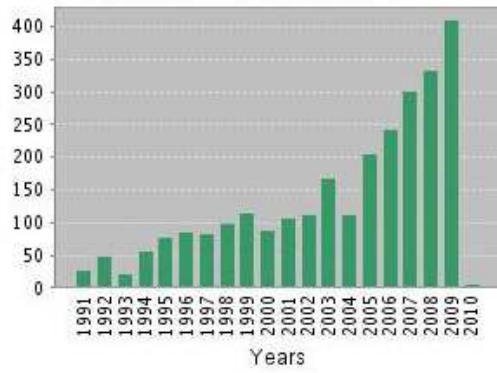
- First prize for bachelor degree in the Faculty of Chemistry in Complutense University.
- First prize for bachelor degree in Chemistry in Spain (for all bachelors in Chemistry of the contry obtained in 1987).
- First prize for PhD degree in the FAculy of Chemistry in Complutense University.
- Since January 2007 I belong to the Editorial Board of Molecular Physics.
- I act as referee for the following journals (7-8 papers/year) Journal of Chemical Physics, Journal of Physical Chemistry, Molecular Physics, J.Phys.Condens.Matter, Ind.Engineering Chemistry Research, Physical Review E, Phys.Rev.Lett. , Fluid Phase Equilibria.
- Fulbright post-doctoral fellowship in the United States during the years 1991 and 1992 (after the supervision of Prof. Peter A. Monson).

Published Items in Each Year



The latest 20 years are displayed.

Citations in Each Year



The latest 20 years are displayed.

Results found: 135

Sum of the Times Cited [?]: 2,716
[View Citing Articles](#)
[View without self-citations](#)

Average Citations per Item [?]: 20.12

h-index [?]: 28

Figura 1: History of papers and citations according to ISI (AUTHOR = VEGA C, ADDRESS= quim fis or fac ciencias QUIM and complutense or amherst or bochum or amsterdam)