

Currículum vitae

Name : Carlos Vega de las Heras

Name : VEGA DE LAS HERAS

First name: CARLOS

National ID Card (Spain)

Genre : Male

Date of birth : 28-8-1964

Bachelor Degree : Chemistry, U.Complutense, 1987.

PhD degree : Chemistry, U.Complutense, 1991 (Prof.S.Lago, PhD advisor) .

Current Position : Full Professor.

University : UNIVERSIDAD COMPLUTENSE

Faculty : FACULTAD DE CIENCIAS QUÍMICAS

Department : DEPARTAMENTO DE QUÍMICA FÍSICA

Address : CIUDAD UNIVERSITARIA, 28040 MADRID

Phone : 34 91 3944202

FAX: 34 91 3944135

e-mail: cvega@quim.ucm.es

-
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).

 5. AUTHORS :T.Boublik, C.Vega, S.Lago y M.D.Peña
 Title: *Quadrupolar hard gaussian*
 Journal: Molec.Phys. **71**, 1193–1203, (1990).

 6. AUTHORS : C.Vega y S.Lago
 Title: *Molecular dynamics study of propane using two simple potential models*
 Journal: J.Chem.Phys. **93**, 8171–8179, (1990).

 7. AUTHORS : C.Vega y S.Lago
 Title: *Structural study of the angle averaged soft Kihara potential for linear molecular models. A test of perturbation theory*
 Journal:Molec.Phys. **72**, 215–228 , (1991).

 8. AUTHORS : C.Vega y S.Lago
 Title: *Perturbation theory of angular Kihara fluids*
 Journal:Journal of Chemical Physics **94**,310–320, (1991)

 9. AUTHORS : P.Sevilla, S.Lago, C.Vega y P.Padilla
 Title: *Solution of the Percus-Yevick equation for linear molecules interacting through either a Kihara or a soft repulsive potential*
 Journal: Phys.Chem.Liq. **23**,1–14, (1991).

 10. AUTHORS : A.Lopez Rodriguez, C.Vega, J.Freire y S.Lago
 Title: *Potential parameters of methylene and methyl group from second virial coefficients of n-alkanes*
 Journal: Molecular Physics **73**, 691–701 (1991).

 11. AUTHORS :P.Padilla, S.Lago y C.Vega
 Title: *A bridge between Fischer and Boublik Thermodynamic perturbationtheory : Calculating thermodynamic properties of pure substances*
 Journal:Molecular Physics **74**, 161–176, (1991).

12. AUTHORS : C.Vega y S.Lago
Title: *Improved perturbation theory of Kihara fluids*
Journal: Chem.Phys.Lett. **185**, 516–521, (1991).

13. AUTHORS : C.Vega
Title: *Perturbation theory of hard quadupolar fluids*
Journal: Molec.Phys. **75**, 427–442, (1992)

14. AUTHORS : C.Vega y K.E.Gubbins
Title: *Monte Carlo study of quadrupolar Kihara fluids*
Journal: Molec.Phys. **75**, 881–895, (1992).

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).

16. AUTHORS : C.Vega, S.Lago, R.Pospisil, S.Labik and A.Malijevsky Title: *Thermodynamic properties of mixtures from perturbation theory* Journal: J.Phys.Chem. **96**, 1895–1899, (1992).

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).

18. AUTHORS : C.Vega, S.Lago, E.de Miguel y L.Rull Title: *Liquid-vapor equilibria of linear Kihara molecules.* Journal: J.Phys.Chem. **96**, 7431–7437, (1992)

19. AUTHORS : E.P.A.Paras, C.Vega y P.A.Monson Title: *Application of the cell theory to the thermodynamic properties of hard dumbbell solids* Journal: Molec.Phys. **77**, 803–821, (1992).

20. AUTHORS : C.Vega, E.P.A.Paras y P.A.Monson Title: *On the stability limit of the plastic crystal phase of hard dumbbell solids* Journal: J.Chem.Phys. **97**, 8543–8548, (1992).

21. AUTHORS : E.P.A.Paras, C.Vega y P.A.Monson Title: *A generalized Van der Waals theory of solid-fluid equilibria for nonspherical molecules.* Journal: Molec.Phys. **79**, 1063–1072, (1993).

22. AUTHORS : C.Vega , R.D.Kaminsky y P.A.Monson Title: *Adsorption of fluids in disordered porous media from integral equation theory* Journal: Journal of Chemical Physics **99**, 3003–3013 (1993).

23. AUTHORS : A.Lopez , C.Vega, J.Freire y S.Lago Title: *Improved results for the potential parameters of methyl and methylene obtained from second virial coefficients of n-alkanes* Journal: Molec.Phys. **80**, 1565–1567, (1993).

24. AUTHORS : C.Vega, S.Lago y B.Garzon Title: *Virial coefficients and equation of state of hard alkane models* Journal: J.Chem.Phys. **100**, 2182–2190, (1994).

25. AUTHORS : C.Vega y S.Lago Title: *A fast algorithm to evaluate the shortest distance between rods* Journal: Computers and Chemistry **18**, 55–59, (1994).

26. AUTHORS : C.Vega y S.Lago Title: *Isotropic-nematic transition of hard polar and nonpolar molecules* Journal: J.Chem.Phys. **100**, 6727–6737, (1994).

27. AUTHORS :S.Lago, J.L.Lopez-Martin, B.Garzon y C.Vega Title: *Vapor-liquid equilibrium from a simple thermodynamic perturbation theory* Journal:J.Phys.Chem. **98**, 5355–5361 , (1994).
-
28. AUTHORS :B.Garzon, S.Lago y C.Vega, E.de Miguel y L.F.Rull Title: *Computer simulation of vapor-liquid equilibria of linear quadrupolar fluids. Departures from the principle of corresponding states* Journal:J.Chem.Phys. **101**, 4166–4176, (1994).
-
29. AUTHORS :C.Vega,S.Lago y B.Garzon Title: *Linear Hard spheres models:Virial coefficients and equation of state* Journal:Molec.Phys. **82**, 1233–1247, (1994).
-
30. AUTHORS :C.Vega, S.Lago y B.Garzon Title: *Liquid vapor equilibria of polar fluids from a van der Waals like theory.* Journal:J.Phys.Chem.**98**,11181-11192,(1994).
-
31. AUTHORS : B.Garzon, S.Lago y C.Vega Title: *Reaction Field simulations of the vapor-liquid equilibria of dipolar fluids : Does the reaction field dielectric constant affect the coexistence properties ?* Journal:Chem.Phys.Lett. **231**,366–372, (1994).
-
32. AUTHORS :C.Vega y P.A.Monson Title: *Solid fluid equilibria for quadrupolar hard dumbbells via Monte Carlo simulation* Journal: J.Chem.Phys. **102**,1361–1372, (1995).
-
33. AUTHORS :P.Padilla y C.Vega Title: *Packing effects on the conformational equilibrium of alkanes* Journal:Molec.Phys. **84**, 435–450, (1995).
-
34. AUTHORS :C.Vega, L.F.Rull y S.Lago Title: *Determination of the Fisher Widom line for systems interacting through short ranged potentials* Journal:Phys.Rev.E. **51**, 3146–3155, (1995).
-
35. AUTHORS :B.Garzon, S.Lago , C.Vega, y L.F.Rull Title: *Computer simulation of vapor-liquid equilibria of linear dipolar fluids. Departures from the principle of corresponding states* Journal:J.Chem.Phys. **102**, 7204–7215, (1995).
-
36. AUTHORS :C.Vega, B.Garzon, L.G.McDowell y S.Lago Title: *The vapour-liquid equilibria of propane and n-alkane conformers* Journal:Molec.Phys. **85**, 679-699, (1995).
-
37. AUTHORS :C.Vega and P.A.Monson Title: *Solid-liquid equilibrium for quadrupolar molecules* Journal:Molec.Phys. **85**,413–421, (1995).
-
38. AUTHORS :A.Gil Villegas, C.Vega, F.del Rio y A.Malijevsky Title: *Structure of variable-width square-well fluids from the Reference Hypernetted Chain equation* Journal: Molec.Phys. **86**,857–864, (1995).
-
39. AUTHORS : C.Vega ,L.G.MacDowell and P.Padilla Title: *Equation of state for hard n-alkane models: Long chains* Journal: Journal of Chemical Physics **104**, 701–713 (1996).
-
40. AUTHORS :L.F.Rull, C.Vega and S.Lago Title: *Absence of criticality in the Reference Hypernetted Chain Equation* Journal:Molec.Phys. **87**, 1235–1242, (1996).
-
41. AUTHORS :A.Gil Villegas, F.del Rio y C.Vega Title: *Thermodynamics of fluids from equivalence of collision properties* Journal: Phys.Rev.E **53**, 2326-2336, (1996).
-

42. AUTHORS :X.Cottin, E.P.A.Paras, C.Vega and P.A.Monson Title: *Fluid-solid Equilibrium : New perspectives from molecular theory* Journal: *Fluid Phase Equilibria* **117**, 114–125, (1996).
-
43. AUTHORS :C.Vega and L.G.MacDowell Title: *Understanding the critical properties of chain molecules* Journal: *Molec.Phys.* **88**,1575–1602, (1996).
-
44. AUTHORS : C.Vega y A.Lopez Rodriguez Title: *Second virial coefficient, critical temperatures and shape of n-alkanes* Journal: *Journal of Chemical Physics* **105**, 4223–4233 (1996).
-
45. AUTHORS :C.Vega, F.Bresme and J.L.F.Abascal Title: *The fluid solid equilibrium of charged hard spheres* Journal: *Phys.Rev.E* **54**, 2746–2760, (1996).
-
46. AUTHORS :C.Vega, B.Garzon, L.G.MacDowell, P.Padilla, S.Calero and S.Lago Title: *The vapour-liquid equilibrium of n-alkanes* Journal:*J.Phys.Condens.Matter* **8**, 9643–9648, (1996).
-
47. AUTHORS : P.Padilla and C.Vega Title: *n-alkanes in random porous media: Can we regard the system as a binary equilibrium mixture ?* Journal: *Journal of Chemical Physics* **106**, 1997–2011 (1997).
-
48. AUTHORS : C.Vega Title: *Virial coefficient and equation of state of hard ellipsoids* Journal:*Molec.Phys.* **92**, 651–665, (1997).
-
49. AUTHORS :C.Vega and P.A.Monson Title: *Plastic Crystal Phases of hard dumbbells and hard spherocylinders* Journal:*J.Chem.Phys.* **107**, 2696–2697,(1997).
-
50. AUTHORS : S. Lago, B.Garzon, S. Calero and C.Vega Title: *Accurate simulations of the vapor-liquid equilibrium of important organic solvents and other diatomics* Journal:*J.Phys.Chem.* **101**, 6763–6771, (1997).
-
51. AUTHORS :C.Vega Title: *The phase diagram of mixtures of hard spheres in the limit of infinite size ratio* Journal:*J.Chem.Phys.* **108**, 3074–3075, (1998).
-
52. AUTHORS :C.Vega, B.Garzon,S.Lago and P.A.Monson Title: *Understanding the phase diagram of quadrupolar fluids* Journal:*J.Mol.Liq.* **76**, 157–169, (1998).
-
53. AUTHORS :P.Padilla, O.Pizio, A.Trokhymchuk and C.Vega Title: *Adsorption of dimerizing and dimmer fluids in disordered porous media* Journal:*J.Phys.Chem.* **102**,3012–3017, (1998).
-
54. AUTHORS : L.G.MacDowell and C.Vega Title: *The second virial coefficient of hard alkane models* Journal: *Journal of Chemical Physics* **109**, 5670–5680, (1998).
-
55. AUTHORS : L.G.MacDowell and C.Vega Title: *Vapour-liquid equilibria of linear and branched alkanes from perturbation theory* Journal: *Journal of Chemical Physics* **109**, 5681–5690, (1998).
-
56. AUTHORS :P.Padilla, C.Vega, O.Pizio and A.Trokhymchuk Title: *The structure and adsorption of diatomic fluids in disordered porous media: A MC study.* Journal: *Molecular Physics* **95** , 701–712, (1998).
-
57. AUTHORS :C.Vega and P.A.Monson Title: *Solid-Fluid equilibrium for a molecular model with short ranged directional forces* Journal:*Journal of Chemical Physics* **109**, 9938–9949 , (1998).
-

58. AUTHORS :B.Garzon, S.Lago, C.Vega. Title: *Monte Carlo simulations of dipolar and quadrupolar linear Kihara fluids. A test of thermodynamic perturbation theory* Journal: *Molecular Physics* **96** , 123–132 , (1999).
-
59. AUTHORS :A.Lopez Rodriguez, C.Vega and J.J.Freire Title: *Determination of potential parameters for alkanes* Journal: *J.Chem.Phys.* **111** , 438–439 , (1999).
-
60. AUTHORS : L.G.MacDowell, C.Vega and A.L.Rodriguez Title: *Critical properties of mixtures of alkanes from perturbation theory* Journal: *J.Chem.Phys.* **111** , 3183–3191 , (1999).
-
61. AUTHORS :C.Vega,L.G.MacDowell and A.L.Rodriguez. Title: *Excess properties of mixtures of n-alkanes from perturbation theory* Journal: *J.Chem.Phys.* **111** , 3192–3202 , (1999).
-
62. AUTHORS :A.P.Malanoski,C.Vega and P.A.Monson Title: *An application of Cell Theory to Molecular Models of n-alkane solids* Journal: *Molecular Physics* **98** , 363–370, (2000).
-
63. AUTHORS :L.G.MacDowell, M.Muller, C.Vega and K.Binder Title: *Equation of state and critical behavior of polymer models: A quantitative comparison between Wertheim's thermodynamic perturbation theory and computer simulations* Journal: *J.Chem.Phys.* **113** , 419–433 , (2000).
-
64. AUTHORS :C.Vega Title: *Evaluating virial coefficients for multicomponent mixtures: hard sphere mixtures and flexible chains* Journal: *Molecular Physics* **98**, 973–985 , (2000).
-
65. AUTHORS :C.Vega and L.G.MacDowell Title: *Critical temperature of infinitely long chains from Wertheim's perturbation theory* Journal: *Molecular Physics* **98** ,1295–1308 , (2000).
-
66. AUTHORS :F.Bresme, C.Vega and J.L.F.Abascal Title: *Order-disorder transition in the solid phase of a charged hard sphere model* Journal: *Phys.Rev.Lett.* **85**, 3217–3220 , (2000).
-
67. AUTHORS :C.Vega, J.M.Labaig, L.G.MacDowell and E.Sanz Title: *The virial coefficients of the pearl-necklace model* Journal: *J.Chem.Phys.* **113** , 10398–10409 , (2000).
-
68. AUTHORS : C.Menduina, C.McBride y C.Vega Title: *The second virial coefficient of quadrupolar two center Lennard-Jones models* Journal: *Physical Chemistry and Chemical Physics* **3** , 1289–1296 , (2001).
-
69. AUTHORS :C.McBride, C.Vega y L.G.MacDowell Title: *Isotropic-nematic transition : a study of the influence of intra-molecular flexibility using a fused hard sphere model.* Journal: *Physical Review E* **64** , 011703-1–011703-14 , (2001).
-
70. AUTHORS :C.Vega y L.G.MacDowell Title: *Extending Wertheim's theory to the solid phase: the freezing of the pearl-necklace model* Journal: *J.Chem.Phys.* **114** , 10411–10418 , (2001).
-
71. AUTHORS :C.Vega ,C.McBride y L.G.MacDowell Title: *Liquid crystal phase formation for the linear tangent hard sphere model from Monte Carlo simulations* Journal: *J.Chem.Phys.* **115** , 4203–4211 , (2001).
-
72. AUTHORS : L.G.MacDowell, C.Vega y E.Sanz Title: *Equation of state of model branched alkanes: theoretical predictions and configurational bias Monte Carlo simulations* Journal: *J.Chem.Phys.* **115** , 6220–6235 , (2001).
-
73. AUTHORS : C.McBride y C.Vega Title: *Fluid-solid equilibrium for two dimensional hard disk chains from Wertheim's perturbation theory* Journal: *Journal of Chemical Physics* **116** , 1757–1759 (2002).
-

74. AUTHORS : C.Vega C.McBride and L.G.MacDowell Title: *The effect of flexibility on the phase diagram of simple molecular models* Journal: *Physical Chemistry and Chemical Physics* **4** , 853–862 (2002).
-
75. AUTHORS : C.Vega,F.J.Blas y A.Galindo Title: *Extending Wertheim's perturbation theory to the solid phase of Lennard-Jones chains. Determination of the global phase diagram.* Journal: *Journal of Chemical Physics* **116** , 7645–7655, (2002).
-
76. AUTHORS : C.Vega,C.McBride Title: *Scaling laws for the equation of state of flexible and linear tangent hard sphere chains.* Journal: *Physical Review E* **65** , 052501–052504, (2002).
-
77. AUTHORS : C.Vega,C.McBride, C.Menduina Title: *The second virial coefficient of the dipolar two center Lennard-Jones model.* Journal: *Physical Chemistry and Chemical Physics* **4** , 3000-3007, (2002).
-
78. AUTHORS : J.Largo, C.Vega , L.G.MacDowell and J.R.Solana Title: *A computer simulation study of racemic mixtures* Journal: *Molecular Physics* **100** , 2397–2415 (2002).
-
79. AUTHORS : E.de Miguel and C.Vega Title: *The global phase diagram of the Gay Berne model* Journal: *Journal of Chemical Physics* , **117** , 6313–6322 (2002).
-
80. AUTHORS : C.McBride and C.Vega Title: *A Monte Carlo study of the influence of molecular flexibility on the phase diagram of a fused hard sphere model* Journal: *Journal of Chemical Physics* ,**117**, 10370–10379, (2002).
-
81. AUTHORS : F.J.Blas,A.Galindo y C.Vega Title: *Study of the solid-liquid-vapor phase equilibria of flexible chain molecules using Wertheim's thermodynamic perturbation theory* Journal: *Molecular Physics* ,**101**, 449–458, 1016 (2003).
-
82. AUTHORS : C.Vega,C.McBride, E.de Miguel, F.J.Blas y A.Galindo Title: *The phase diagram of the two center Lennard-Jones model as obtained from computer simulation and from Wertheim's thermodynamic perturbation theory* Journal: *Journal of Chemical Physics* ,**118**, 10696–10706, (2003).
-
83. AUTHORS : L.G.MacDowell,C.Menduina, C.Vega y E.de Miguel Title: *The third virial coefficient of diatomic quadrupolar molecules* Journal: *Physical Chemistry and Chemical Physics*, 2851–2857,(2003).
-
84. AUTHORS : C.Vega,J.L.F.Abascal, C.McBride, y F.Bresme Title: *The fluid-solid equilibrium for a charged hard sphere model revisited* Journal: *Journal of Chemical Physics* ,**119**, 964–971, (2003).
-
85. AUTHORS : E.Sanz, C.McBride y C.Vega Title: *The properties of fully flexible Lennard-Jones chains in the solid phase: Wertheim's TPT1 theory and simulation.* Journal: *Molecular Physics*, **101**, 2241-2255, (2003).
-
86. AUTHORS : J.Largo,M.J.Maeso,J.R.Solana, C.Vega y L.G.MacDowell Title: *Bonded hard-sphere theory and computer simulation of the equation of state of linear fused hard sphere fluids.* Journal: *Journal of Chemical Physics*, **119**,9633–9639,(2003).
-
87. AUTHORS : F.J.Blas, E.Sanz, C.Vega y A.Galindo Title: *Fluid-solid equilibria of flexible and linear rigid tangent chains from Wertheim's thermodynamic perturbation theory* Journal: *Journal of Chemical Physics* , **119**, 10958–10971, (2003).
-
88. AUTHORS : L.G.MacDowell,C.Menduina, C.Vega y E.de Miguel Title: *Critical properties of molecular fluids from the virial series* Journal: *Journal of Chemical Physics* , **119**, 11367–11373, (2003).
-

89. AUTHORS : J.L.F.Abascal, C.Vega, C.McBride y F.Bresme , Title: *Characterization of the order-disorder transition of a charged hard sphere model* Journal: *Physical Review E* , **68**, 052501–052504, (2003)
-
90. AUTHORS : C.Vega,L.G.MacDowell, C.MacBride, E.Sanz, F.J.Blas y A.Galindo Title: *Molecular modeling of flexible molecules: vapor-liquid and fluid-solid equilibria.* Journal: *Journal of Molecular Liquids* ,**113**, 37–51, ,(2004).
-
91. AUTHORS : A.Galindo, C.Vega, E.Sanz, L.G.MacDowell, E.de Miguel y F.J.Blas Title: *Computer simulation study of the global phase behaviour of linear rigid Lennard-Jones chain molecules: Comparison with flexible model* Journal: *J.Chem.Phys.* ,**120**, 3957–3968, (2004).
-
92. AUTHORS : E.Sanz,C.Vega, J.L.F.Abascal and L.G.MacDowell Title: *The phase diagram of water from computer simulation* Journal: *Physical Review Letters* ,**92**, 255701,(2004).
-
93. AUTHORS : E.Sanz,C.Vega, J.L.F.Abascal and L.G.MacDowell Title: *Tracing the phase diagram of the TIP4P model of water* Journal: *J. Chem. Phys.* **121**, 1165-1166 (2004).
-
94. AUTHORS : L.G.MacDowell, E.Sanz, C.Vega and J.L.F.Abascal Title: *Combinatorial entropy and phase diagram of partially ordered ice phases* Journal: *J. Chem. Phys.* **121**, 10145-10158 (2004).
-
95. AUTHORS : Carl Mc Bride, Carlos Vega, Eduardo Sanz, Jose L. F. Abascal Title: *Formation of high density amorphous ice by decompression of ice VII and ice VIII at 135 K.* Journal: *J. Chem. Phys.* **121**, 11907–11911 (2004).
-
96. AUTHORS : C.McBride,C.Vega, E.Sanz,C.Vega, J.L.F.Abascal y L.G.MacDowell Title: *The range of meta stability of ice-water melting for two simple models of water* Journal: *Molecular Physics* , **103**, 1–5, (2005).
-
97. AUTHORS : C.Vega, E.Sanz y J.L.F.Abascal Title: *The melting point of the most popular models of water* Journal: *Journal of Chemical Physics* , **122**,114507, (2005).
-
98. AUTHORS : C.Vega, C.McBride, E.Sanz, J.L.F.Abascal Title: *Radial distrubution 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* Journal: *Physical Chemistry Chemical Physics* , **7**,1450–1456, (2005).
-
99. AUTHORS : J.L.F.Abascal, E.Sanz, R.Garcia y C.Vega Title: *A potential model for the study of ices and amorphous water: TIP4P/Ice* Journal: *Journal of Chemical Physics* , **122**,234511, (2005).
-
100. AUTHORS : C.McBride, C.Vega, y E.Sanz Title: *Non-Markovian melting: a novel procedure to generate initial liquid like phases for small molecules for use in computer simulation studies.* Journal: *Computer Physics Communications* , **170**, 137–143, (2005).
-
101. AUTHORS : C.Vega y J.L.F.Abascal Title: *Relation between the melting temperature and the temperature of maximum density for the most common models of water* Journal: *Journal of Chemical Physics* , **123**, 144504, (2005).
-
102. AUTHORS : C.Vega , J.L.F.Abascal, E.Sanz, L.G.MacDowell y C.McBride Title: *Can simple models describe the phase diagram of water ?* Journal: *Journal of Physics Condensed Matter* , **17**, S3283–S3288, (2005).
-
103. AUTHORS : J.L.F.Abascal y C.Vega Title: *A general purpose model for the condensed phases of water: TIP4P/2005* Journal: *Journal of Chemical Physics* , **123**, 234505, (2005).
-

104. AUTHORS : R.G.Fernandez, J.L.F.Abascal y C.Vega Title: *The melting point of ice I_h for common water models calculated from direct coexistence of the solid-liquid interface* Journal: Journal of Chemical Physics , **124**, 144506, (2006).
-
105. AUTHORS : C.Vega, J.L.F.Abascal y I.Nezbeda Title: *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* Journal: Journal of Chemical Physics , **125**, 034503, (2006).
-
106. AUTHORS : H.Docherty, A.Galindo, C.Vega y E.Sanz Title: *A potential model for methane in water describing correctly the solubility of the gas and the properties of the methane hydrate* Journal: Journal of Chemical Physics , **125**, 074510, (2006).
-
107. AUTHORS : M.Martin-Conde, C.Vega y L.G.MacDowell Title: *Computer simulation of two new solid phases of water: ice XIII and ice XIV* Journal: Journal of Chemical Physics , **125**, 116101, (2006).
-
108. AUTHORS : J.L.F. Abascal, R.G. Fernandez, C.Vega y M.A.Carignano Title: *The melting temperature of the six site potential model of water* Journal: Journal of Chemical Physics , **125**, 166101, (2006).
-
109. AUTHORS (p.o. de firma): C. Vega and P. A. Monson TITLE: *Solid-fluid equilibrium for a molecular model with short ranged directional forces (erratum)* JOURNAL: Journal of Chemical Physics , **125**, 109901-1,109901-2, (2006).
CLAVE: A
-
110. AUTHORS : C.Vega , M.Martin-Conde y A.Patrykiewicz Title: *Absence of superheating for ice I_h with a free surface: a new method of determining the melting point of different water models.* Journal: Molecular Physics , **104**, 3583–3592 (2006).
-
111. AUTHORS : E.Sanz y C.Vega TITLE: *Solubility of KF and NaCl in water by molecular simulation* JOURNAL: J.Chem.Phys. , **126**, 014507, (2007) .
-
112. AUTHORS : C.Vega y E.de Miguel TITLE: *The surface tension of the most popular models of water by using the extended Widom method* JOURNAL: J.Chem.Phys. , **126**, 154707, (2007).
-
113. AUTHORS : J.L.F.Abascal y C.Vega TITLE: *The melting point of hexagonal ice (I_h) is strongly dependent on the quadrupole of the water models* JOURNAL: Physical Chemistry Chemical Physics , **9**, 2775-2778 , (2007).
-
114. AUTHORS : J.L.F.Abascal y C.Vega TITLE: *Dipole-Quadrupole force ratios determine the ability of potentials models to describe the phase diagram of water* JOURNAL: Physical Review Letters , **98**, 237801 , (2007).
-
115. AUTHORS : H.Docherty, A.Galindo, C.Vega y E.Sanz TITLE: *An investigation of the salting out of methane from aqueous electrolyte solutions using computer simulations* JOURNAL: J.Phys.Chem.B , **111**, 8993-9000, (2007).
-
116. AUTHORS : E.G.Noya, C.Vega , J.P.K.Doye and A.A.Louis TITLE: *Phase diagram of model anisotropic particles with octahedral symmetry* JOURNAL: J.Chem.Phys. , **127**, 054501, (2007).
-
117. AUTHORS : J.L.Aragones, J.L.F.Abascal, E.G.Noya y C.Vega TITLE: *Properties of ices at 0 K: a test of water models* JOURNAL: J.Chem.Phys. , **127**, 154518 , (2007).
-
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).
-

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).
-
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).
-
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).
-
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).
-
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).
-
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).
-
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).
-
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).
-
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).
-
131. AUTHORS (p.o. de firma): H.L.Pi, J.L.Aragones, C.Vega, E.G.Noya, J.L.Abascal , M.A.Gonzalez and C.McBride TITLE: *Anomalies in water as obtained from computer simulations of the TIP4P/2005 model: density maxima, and density, isothermal compressibility and heat capacity minima* JOURNAL: Molec. Phys. , 107, 365, (2009).
-
132. AUTHORS (p.o. de firma): J.L.Aragones y C.Vega TITLE: *Plastic crystal phases of simple water models* JOURNAL: J.Chem.Phys. , 130, 244504, (2009).
-

133. AUTHORS (p.o. de firma): C.McBride,C.Vega,E.G.Noya,R.Ramirez and L.M.Sese TITLE: *Quantum contribution in the ice phases: the path to a newempirical model for water: TIP4PQ/2005* JOURNAL: J.Chem.Phys. , 131, 024506 , (2009).
-
134. AUTHORS (p.o. de firma): M.M.Conde, C. Vega, G.A.Tribello and B.Slater TITLE: *The phase diagram of water at negative pressures: Virtual ices* JOURNAL: J.Chem.Phys. , 131, 034510 , (2009).
-
135. AUTHORS (p.o. de firma): E.G.Noya ,C.Vega, L.M.Sese y R.Ramirez TITLE: *Quantum effects on the maximum in density of water as described by the TIP4PQ/2005 model* JOURNAL: J.Chem.Phys. , 131 124518 (2009) .
-
136. AUTHORS (p.o. de firma): C.Vega , M. M. Conde , C. McBride , J.L.F. Abascal , E.G. Noya , R.Ramirez y L.M.Sese TITLE: *Heat capacity of water: a signature of nuclear quantum effects* JOURNAL: J.Chem.Phys. , 132, 046101 (2010) .
-
137. AUTHORS (p.o. de firma): B. Gonzalez , E.G.Noya , C. Vega y L. M. Sese TITLE: *Nuclear Quantum Effects in Water Clusters: The Role of the Molecular Flexibility* JOURNAL: J.Phys.Chem. B , 114, 2484-2492 (2010).
-
138. AUTHORS (p.o. de firma): D.G.Salgado y C. Vega TITLE: *Melting point and phase diagram of methanol as obtained from computer simulations of the OPLS model* JOURNAL: J.Chem.Phys. , 132 , 094505 , (2010).
-
139. AUTHORS (p.o. de firma): M. M. Conde, C.Vega, C. McBride, E.G.Noya, R.Ramirez y L. M. Sese TITLE: *Can gas hydrate structures be described using classical simulations?* JOURNAL: J.Chem.Phys. , 132, 114503 , (2010).
-
140. AUTHORS (p.o. de firma): L. G. MacDowell y C. Vega TITLE: *Dielectric Constant of Ice Ih and Ice V: A Computer Simulation Study* JOURNAL: J. Phys. Chem. B, , 114, 6089, (2010).
-
141. AUTHORS (p.o. de firma): E.G.Noya, C.Vega , J.P.K.Doye and A.A.Louis TITLE: *The stability of a crystal with diamond structure for patchy particles with tetrahedral symmetry* JOURNAL: J.Chem.Phys. , 132, 234511 , (2010).
-
142. AUTHORS (p.o. de firma): M. M. Conde and C. Vega TITLE: *Determining the three-phase coexistence line in methane hydrates using computer simulations* JOURNAL: J. Chem. Phys. , 133, 064507, (2010).
-
143. AUTHORS (p.o. de firma): J. L. F. Abascal and C. Vega TITLE: *Widom line and the liquid-liquid critical point for the TIP4P/2005 water model* JOURNAL: J. Chem. Phys. , 133, 234502 , (2010).
-
144. AUTHORS (p.o. de firma): E.G.Noya,L.M.Sese,R.Ramirez,C.McBride, M.M.Conde and C.Vega TITLE: *Path integral Monte Carlo simulations for rigid rotors and their application to water* JOURNAL: Molecular Physics , 109, 149-168 , (2011).
-
145. AUTHORS (p.o. de firma): E.G.Noya, C. Vega and C.McBride TITLE: *A quantum propagator for path-integral simulations of rigid molecules* JOURNAL: J. Chem. Phys. , 134, 054117 , (2011).
-
146. AUTHORS : L.J.Bonales , J.E.F.Rubio, H.Ritacco, C.Vega, R.G.Rubio and F.Ortega TITLE: *Freezing transition and interaction potential in monolayers of microparticles at fluid interfaces* JOURNAL: Langmuir , 27, 3391-3400, , (2011).
-

147. AUTHORS : D.G.Salgado, A.Dopazo-Paz, P.Gomez-Alvarez , J.M.Miguez y C. Vega TITLE: *Solid-solid and solid-fluid equilibria of the most popular models of methanol obtained by computer simulation* JOURNAL: J. Phys.Chem.B , 115, 3522-3530 , (2011).
-
148. AUTHORS : J. L. F Abascal and C. Vega TITLE: *Equation of state and compressibility of supercooled water: simulations and experiment* JOURNAL: J. Chem. Phys. 134 186101 , (2011).
-
149. AUTHORS : J. L. Aragonés , L. G. MacDowell y C. Vega TITLE: *Dielectric constant of ices and water : a lesson about water interactions* JOURNAL: J. Phys.Chem.A , 115, 5745 , (2011).
-
150. AUTHORS : J. L. Aragonés , L. G. MacDowell, I. J. Siepmann and C. Vega TITLE: *Phase diagram of water under an applied electric field* JOURNAL: Physical Review Letters , 107, 155702 , (2011).
-
151. AUTHORS : C. Vega and J. L. F. Abascal TITLE: *Simulating water with rigid non-polarizable models: a general perspective* JOURNAL: Physical Chemistry Chemical Physics , 13, 19663 , (2011).
-
152. AUTHORS : C. Vega , J. L. F. Abascal and P. G. Debenedetti TITLE: *Physics and Chemistry of Water and Ice* JOURNAL: Physical Chemistry Chemical Physics , 13, 19660 , (2011).
-
153. AUTHORS : J. L. Aragonés , E. Sanz and C. Vega TITLE: *Solubility of NaCl in water by molecular simulation revisited* JOURNAL: Journal of Chemical Physics , 136, 244508 , (2012).
-
154. AUTHORS : C.McBride , E.G. Noya , J.L. Aragonés , M. M. Conde and C. Vega TITLE: *The phase diagram of water from quantum simulations* JOURNAL: Physical Chemistry Chemical Physics , 14, 10140 , (2012).
-
155. AUTHORS : J. L. Aragonés , E. Sanz, C. Valeriani and C. Vega TITLE: *Calculation of the melting point of alkali halides by means of computer simulations* JOURNAL: Journal of Chemical Physics , 137, 104507 , (2012).
-
156. AUTHORS : C.McBride , J.L. Aragonés , E.G. Noya y C. Vega TITLE: *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* JOURNAL: Physical Chemistry Chemical Physics , 14, 15199 , (2012).
-
157. AUTHORS : J. L. Aragonés , C. Valeriani and C. Vega TITLE: *Free energy calculations for atomic solids through the Einstein crystal/molecule methodology using GROMACS and LAMMPS* JOURNAL: Journal of Chemical Physics , 137, 146101 , (2012).
-
158. AUTHORS : A. Reinhardt, J.P.K.Doye, E.G. Noya y C. Vega TITLE: *Local order parameters for use in driving homogeneous ice nucleation with all-atom models of water* JOURNAL: Journal of Chemical Physics , 137, 194504 , (2012).
-
159. AUTHORS : G. Jimenez-Serratos , C. Vega y A. Gil-Villegas TITLE: *Evaluation of the pressure tensor and surface tension for molecular fluids with discontinuous potentials using the volume perturbation method* JOURNAL: Journal of Chemical Physics , 137, 204104 , (2012).
-
160. AUTHORS : C. Vega and S. Sokolowski TITLE: *Orest Pizio: scientist and friend Foreword* JOURNAL: CONDENSED MATTER PHYSICS , 15, 20101 , (2012).
-
161. AUTHORS : M.M.Conde y C. Vega TITLE: *A simple correlation to locate the three phase coexistence line in methane hydrate simulations* JOURNAL: Journal of Chemical Physics , 138, 056101 , (2013).
-

162. AUTHORS : G. Perez-Sanchez, D.Gonzalez-Salgado, M.M.Pineiro y C.Vega TITLE: *Fluid-solid equilibrium of carbon dioxide as obtained from computer simulations of several popular potential models: The role of the quadrupole* JOURNAL: Journal of Chemical Physics , 138, 084506 , (2013).
-
163. AUTHORS : C. McBride, E.G.Noya y C. Vega TITLE: *A computer program to evaluate the NVM propagator for rigid asymmetric tops for use in path integral simulations of rigid bodies* JOURNAL: Computer Physics Communications , 184, 885 , (2013).
-

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 electrolytes 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 hydrocarbons: results for linear carbon skeleton and some hints for non-linear

Contribution : Poster

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

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, Snowbird

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.

62. AUTHORS: 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: Poster , Minneapolis, Mayo 2009.

CONGRESS : Workshop, Molecular Simulations: Algorithms, Analysis, and Applications

63. AUTHORS: C.Vega, J.L.F.Abascal, L.G.MacDowell, M.M.Conde, J.L.Aragones, E.G.Noya y C.McBride

Title: Cinco años simulando el diagrama de fases del agua. Qué hemos aprendido ?

Contribution: Presentacion oral.

CONGRESS : Fisica Estadistica 2009 , Huelva Septiembre, 2009.

Place: Huelva , España.

64. AUTHORS: C.Vega, J.L.F.Abascal, L.G.MacDowell, M.M.Conde, J.L.Aragones, E.G.Noya y C.McBride

Title: Five years simulating the phase diagram of water. What we learn something ?

Contribution: Talk.

CONGRESS : Thermodynamics 2009 , Septiembre, 2009.

Place: Londres, Reino Unido.

65. AUTHORS: C.Vega

Title: Can we describe water using computer simulations ?

Contribution: Invited Lecture (Physical Chemistry Department).

CONGRESS : Universidad de Oxford, Mayo, 2010.

Place: Oxford, UK.

66. AUTHORS: C.Vega

Title: Can we describe water using computer simulations ?

Contribution: Invited Lecture (Faculty of Physics).

CONGRESS : Universidad de Roma, La Sapienza, Enero, 2010.

Place: Roma, Italia.

67. AUTHORS: C.Vega

Title: Describing water using simple models.

Contribution: Invited Lecture (Faculty of Physics).

CONGRESS : Universidad de Luxemburgo, Junio 2010.

Place: Luxemburgo

68. AUTHORS: Carlos Vega.

Title: Crystallisation studies of water: modelling , crystal growth and nucleation

Contribution: Talk.

CONGRESS : Cecam workshop Crystallization: from colloids to pharmaceuticals, Julio, 2010.

Place: Lausanne, Suiza.

69. AUTHORS: J. L. F. Abascal , M. A. Gonzalez and Carlos Vega.

Title: Propiedades del agua en condiciones extremas: región subenfriada y presiones negativas

Contribution: Poster.

CONGRESS : FISES 2011, JUNIO , 2011.

Place: Barcelona.

70. AUTHORS: Carlos Vega.

Title: **Properties of supercooled water as obtained from computer simulations of the TIP4P/2005 model** Contribution: **Talk**

CONGRESS : **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** , Julio, 2011.

Place: **Lausanne, Suiza.**

71. AUTHORS: **Jose Luis F. Abascal , Carlos Vega y Miguel Angel González.**

Title: **Supercooled water: simulation and experiment** Contribution: **Talk**

CONGRESS : **8th Liquid Matter Conference, Septiembre 2011**

Place: **Viena, Austria.**

72. AUTHORS: **Carlos Vega .**

Title: **Computer simulations of water** Contribution: **Invited lecture.**

CONGRESS : **Universidad de Freiburg**

Place: **Freiburg, Alemania, Marzo 2012.**

73. AUTHORS: **Carlos Vega .**

Title: **Computer simulations of the phase diagram of water** Contribution: **Invited talk**

CONGRESS : **Congreso: Statistical Physics: Modern Trends and Applications** , Julio 2012.

Place: **Lviv, Ucrania.**

74. AUTHORS: **Carlos Vega .**

Title: **Computer simulations studies of water** Contribution: **Invited talk**

CONGRESS : **Imperial College, Londres, Marzo 2013.**

Place: **Loncres, Reino Unido.**

75. AUTHORS: **Carlos Vega .**

Title: **Simulating water with rigid non-polarizable models** Contribution: **Invited talk.**

CONGRESS : **University of Wisconsin, Mayo 2013.**

Place: **Madison, Estados Unidos.**

76. AUTHORS: **Carlos Vega .**

Title: **The phase diagram of water as obtained from computer simulations** Contribution: **Charla invitada.**

CONGRESS : **PPEPPD , Mayo 2013 .**

Place: **Iguazu, Argentina.**

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**

Title : **SIMULACIÓN DEL EQUILIBRIO DE FASES DEL AGUA: HIELO E HIDRATOS**

PhD student: **MARÍA MARTÍN CONDE**

University : **Universidad Complutense**

Faculty/School: **Ciencias Químicas**

Title : **SIMULACIÓN DEL EQUILIBRIO DE FASES DEL AGUA: CRISTALES PLÁSTICOS, CONSTANTES DIELÉCTRICAS Y DISOLUCIONES**

PhD student : **JUAN LUIS ARAGONÉS GÓMEZ**

University : **Universidad Complutense**

Faculty/School : **Ciencias Químicas**

Publications analysis.

Journal (impact factor)	Number
Physical Review Letters(6)	4
Faraday Discussion (5)	1
Langmuir (4.5)	1
Journal of Chemical Physics (3.3)	75
Journal of Physical Chemistry (4)	6
Journal of Physical Chemistry B (3.6)	5
Journal of Physical Chemistry C (2)	2
Journal of Physical Chemistry A (2.5)	1
Physical Chemistry and Chemical Physics (3.5)	9
Physical Review E (2.1)	6
Chemical Physics Letters (2.3)	2
Molecular Physics (1.75)	32
Computer Physics Communications (1.51)	2
J.Phys.Condens.Matter(1.8)	3
Fluid Phase Equilibria(0.8)	1
Journal of Molecular Liquids (1.0)	3
Computers and Chemistry (0.8)	2
Physics and Chemistry of Liquids (0.5)	1
Total number of published papers :	163

Citation analysis, updated , May 2013.

Total number of citations : 4510

Papers with more than 100 citations : 9

H (h-index) = 37

Algorithm search for ISI :

AUTHOR: VEGA C

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

Research ID (Web of Science) : 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).

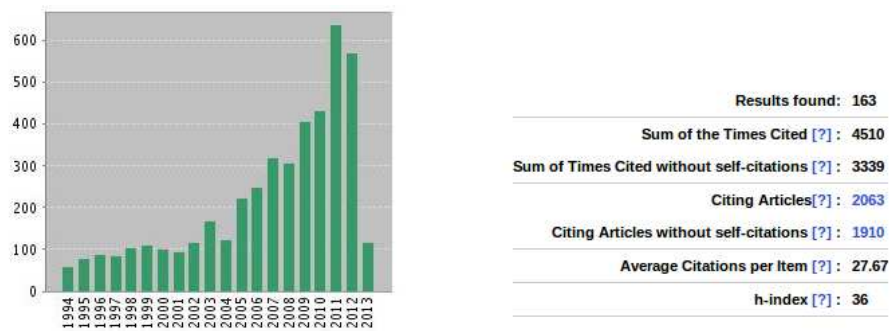


Figura 1: History of papers and citations according to ISI (AUTHOR = VEGA C, ADDRESS= quim fis or fac ciencias QUIM and complutense or amherst or bochum or amsterdam)