

# **Currículum vitae**

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Bachelor Degree : Chemistry, U.Complutense, 1987.

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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).

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  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).

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  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).

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  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).

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  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).

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

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  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).

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  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).

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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).

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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).

---
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 : S.Calero,S.Lago,L.G.MacDowell, B.Garzon y C.Vega. Title: *Simulacion de propiedades dinamicas y de transporte para fluidos lineales de Kihara. Resultados preliminares.* Journal:*Informacion Tecnologica* **8**, 185–191, (1997).
- 
52. 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).
- 
53. 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).
- 
54. 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).
- 
55. AUTHORS :L.G.MacDowell,C.Vega and P.Padilla Title: *Second virial coefficients and equation of state of hard flexible molecules* Journal:*Anales de Fisica* **10**, 1–2, (1998).
- 
56. 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).
- 
57. 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).
-

58. 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).
- 
59. 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).
- 
60. 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).
- 
61. 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).
- 
62. 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).
- 
63. 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).
- 
64. 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).
- 
65. 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).
- 
66. AUTHORS :C.Vega Title: *Evaluating virial coefficients for multicomponent mixtures: hard sphere mixtures and flexible chains* Journal: *Molecular Physics* **98**, 973–985 , (2000).
- 
67. 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).
- 
68. 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).
- 
69. 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).
- 
70. 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).
- 
71. 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).
- 
72. 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).
- 
73. 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).
-

74. 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).
- 
75. 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).
- 
76. 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).
- 
77. 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).
- 
78. 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).
- 
79. 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).
- 
80. 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).
- 
81. 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).
- 
82. 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).
- 
83. 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).
- 
84. 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 from Wertheim's thermodynamic perturbation theory* Journal: *Journal of Chemical Physics* ,**118**, 10696–10706, (2003).
- 
85. 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).
- 
86. 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).
- 
87. 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).
- 
88. 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).
-



89. 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).
- 
90. 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).
- 
91. 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)
- 
92. AUTHORS : C.Vega,L.G.MacDowell, C.McBride, 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).
- 
93. 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).
- 
94. 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).
- 
95. 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).
- 
96. 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).
- 
97. 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).
- 
98. 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).
- 
99. 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).
- 
100. AUTHORS : C.Vega, C.McBride, E.Sanz, J.L.F.Abascal Title: *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* Journal: Physical Chemistry Chemical Physics , **7**,1450–1456, (2005).
- 
101. 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).
- 
102. 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).
- 
103. 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).
-

104. 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).
- 
105. 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).
- 
106. 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).
- 
107. 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).
- 
108. 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).
- 
109. 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).
- 
110. 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).
- 
111. 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).
- 
112. AUTHORS : E.Sanz y C.Vega TITLE: *Solubility of KF and NaCl in water by molecular simulation* JOURNAL: J.Chem.Phys. , **126**, 014507, (2007) .
- 
113. 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).
- 
114. 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).
- 
115. 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).
- 
116. 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).
- 
117. 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).
- 
118. 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).
-

119. 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).
- 
120. 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<sub>h</sub>, II, III, V and VI, as obtained from computer simulation* JOURNAL: J.Phys.Chem.B , **111**, 15877-15888 , (2007).
- 
121. 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).
- 
122. 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).
- 
123. 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).
- 
124. 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).
- 
125. 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).
- 
126. 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).
- 
127. 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).
- 
128. 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).
- 
129. 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).
- 
130. 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).
- 
131. 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).
- 
132. 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. , **xx**, enviado , (2009).
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## 12. Conferences

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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

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

Title: A bridge between Fischer and Boublik thermodynamic perturbation theories

Participation : Poster

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

Place : Merseburg, Alemania

DATE : Agosto 1988

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

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

Participation : Invited Talk

CONGRESS : Internacional. 10th IUPAC Conference on Chemical Thermodynamics

Place : Praga, Checoslovaquia

DATE : Agosto 1988

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4. AUTHORS: C.Vega y D.Frenkel

Title: Monte Carlo study of rod like Kihara molecules

Participation : Talk

CONGRESS : Internacional. NATO ASI

LUGAR DE CELEBRACIÓN: Bath, Reino Unido

DATE : Septiembre 1988

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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

Participation : Poster

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

Place : Santiago de Compostela, España

DATE : Septiembre 1989

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

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

Participation : Poster

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

Place : Praga, Checoslovaquia

DATE : Mayo 1990

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

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

Participation : Poster

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

Place : Lyon, Francia

DATE : Julio 1990

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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

Participation : Poster

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

Place : Southampton, Reino Unido

DATE : Diciembre 1991

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

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

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11. AUTHORS: C.VEGA, E.P.A.PARAS Y P.A.MONSON  
Title: **SOLID-FLUID EQUILIBRIA IN SYSTEMS OF HARD DIATOMICS**  
Participation : **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  
TIPO DE PARTICIPACIÓN: Poster  
CONGRESS : Nacional. XXXV congreso de la Sociedad Mexicana de Física  
Place :Puebla, México  
DATE : Octubre 1992

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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  
TIPO DE PARTICIPACIÓN: Poster  
CONGRESS : Nacional. Física Estadística 93  
Place :El Escorial, Madrid  
DATE : Mayo 1993

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

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

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

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

Place : ZARAGOZA  
AÑO: 1996

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**18. AUTHORS: C.VEGA**

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

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

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

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**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  
Participation : Talk invitada  
CONGRESS : *Internacional. 10th Nordic Symposium on Computer Simulation*  
Place : Tallin, Estonia  
DATE : Julio 1996

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

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

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

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

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

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

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

Title: Vapor-Liquid equilibrium of linear and branched alkanes  
TIPO DE PARTICIPACIÓN: Poster  
CONGRESS : *Internacional. European Molecular Liquids Conference*  
LUGAR DE CELEBRACIÓN: Mureau, Austria  
DATE : Noviembre 1998

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**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  
TIPO DE PARTICIPACIÓN: Poster  
CONGRESS : *Internacional. Thermodynamics 99*  
LUGAR DE CELEBRACIÓN: Londres, Reino Unido  
DATE : Marzo 1999

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

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

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

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

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

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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  
TIPO DE PARTICIPACIÓN: Comunicación oral  
CONGRESS : Internacional. Thermodynamics 2001  
LUGAR DE CELEBRACIÓN:Bristol, Reino Unido.  
DATE : Abril 2001.

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

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

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

TIPO DE PARTICIPACIÓN: **Talk invitada**  
CONGRESS : **Internacional. 17th IUPAC Conference on Chemical Thermodynamics**  
LUGAR DE CELEBRACIÓN: **Rostock, Alemania**  
DATE : **Agosto 2002**

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35. AUTHORS: **C.Vega**  
Title: **The phase diagram of the restricted primitive model**  
TIPO DE PARTICIPACIÓN: **Talk invitada**  
CONGRESS : **Internacional. Thermodynamics 2003 (Royal Society of Chemistry)**  
LUGAR DE CELEBRACIÓN: **Cambridge, United Kingdom.**  
DATE : **Abril, 2003.**

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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**  
TIPO DE PARTICIPACIÓN: **Talk**  
CONGRESS : **Internacional. 15th SYMPOSIUM ON THERMOPHYSICAL PROPERTIES**  
LUGAR DE CELEBRACIÓN: **Boulder, Colorado, USA.**  
DATE : **Junio , 2003.**

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37. AUTHORS: **L.G.MacDowell, C.McBride, C.Menduiña, E.Sanz y C.Vega**  
Title: **Simulación por ordenador de fluidos moleculares**  
TIPO DE PARTICIPACIÓN: **Talk**  
CONGRESS : **Nacional. Primera reunión de expertos en fluidos comprimidos**  
LUGAR DE CELEBRACIÓN: **Madrid, Campo de las Naciones.**  
DATE : **12-14 Noviembre 2003.**

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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**  
TIPO DE PARTICIPACIÓN: **Poster**  
CONGRESS : **Internacional. SAFT Simposium.**  
LUGAR DE CELEBRACIÓN: **Barcelona.**  
DATE : **12 Diciembre 2003.**

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39. AUTHORS: **J.L.F.Abascal, E.Sanz, L.G.MacDowell and C.Vega**  
Title: **Computer simulation of the phase diagram of water**  
TIPO DE PARTICIPACIÓN: **Talk invitada**  
CONGRESS : **Internacional. Statphys 22.**  
LUGAR DE CELEBRACIÓN: **Bangalore, India.**  
DATE : **5-9 Julio 2004**

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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.**  
TIPO DE PARTICIPACIÓN: **Poster.**  
CONGRESS : **Internacional. Conference on Disorder, complexity and Biology (DISCOMBO4).**  
LUGAR DE CELEBRACIÓN: **Varanasi, India.**  
DATE : **12-15 Julio 2004**

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41. AUTHORS: **E.Sanz, C.Vega, J.L.F.Abascal and L.G.MacDowell**  
Title: **The phase diagram of water from computer simulation**  
TIPO DE PARTICIPACIÓN: **Poster**  
CONGRESS : **Internacional. SIMU, bridging the scales.**  
LUGAR DE CELEBRACIÓN: **Genova, Italia.**  
DATE : **29-31 Agosto 2004.**

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



LUGAR DE CELEBRACIÓN: Utah, USA  
DATE : 16-21 May 2004

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**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**  
TIPO DE PARTICIPACIÓN: **Talk**  
CONGRESS : **Thermodynamics 2005 (organizado por la Royal Society of Chemistry)**  
LUGAR DE CELEBRACIÓN: **Sesimbra, Portugal**

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**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**  
TIPO DE PARTICIPACIÓN: **Talk**  
CONGRESS : **6th Liquid Matter Conference (organizado por la European Physical Society) , Julio 2005**  
LUGAR DE CELEBRACIÓN: **Utrecht, Holanda**

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**45. AUTHORS: C.Vega**  
Title: **The phase diagram of water by computer simulation**  
TIPO DE PARTICIPACIÓN: **Talk**  
CONGRESS : **7th Liblice Conference on the Statistical Mechanics of Liquids, Junio 2006**  
LUGAR DE CELEBRACIÓN: **Lednice, Republica Checa**

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**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**  
TIPO DE PARTICIPACIÓN: **Talk**  
CONGRESS : **Cecam workshop. Patchy colloids, Proteins and Network forming liquids: Analogies and new insights from computer simulations , Junio 2006.**  
LUGAR DE CELEBRACIÓN: **Lyon, Francia**

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**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**  
TIPO DE PARTICIPACIÓN: **Poster**  
CONGRESS : **FOMMS (Foundations of Molecular Modeling and Simulation), Julio 2006**  
LUGAR DE CELEBRACIÓN: **Washington, Estados Unidos.**

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**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**  
TIPO DE PARTICIPACIÓN: **Talk**  
CONGRESS : **EMLG/JMLG Annual Meeting, Liquids systems under extreme conditions , Septiembre 2006**  
LUGAR DE CELEBRACIÓN: **Barcelona**

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**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**  
TIPO DE PARTICIPACIÓN: **Talk plenaria invitada.**  
CONGRESS : **CCP5 Annual meeting, Septiembre del 2006.**  
LUGAR DE CELEBRACIÓN: **Bradford, Reino Unido**

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THESIS SUPERVISED AND FINISHED SUCCESSFULLY

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Title: **TERMODINAMICA ESTADISTICA DE MOLECULAS FLEXIBLES: TEORIA Y SIMULACION**

PhD Student : **LUIS GONZÁLEZ MACDOWELL**

University : **Universidad Complutense**

Faculty/School : **Ciencias Químicas**

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Title: **EQUILIBRIO TERMODINÁMICO DE SÓLIDOS MEDIANTE SIMULACIÓN MOLECULAR**

Student : **EDUARDO SANTIAGO SANZ GARCIA**

University : **Universidad Complutense**

Faculty/School : **Ciencias Químicas**

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**Publications analysis.**

<b>Journal (impact)</b>	<b>Number of papers</b>
Physical Review Letters(6)	3
Faraday Discussion (5)	1
Journal of Chemical Physics (3.3)	59
Journal of Physical Chemistry (4)	9
Physical Review E (2.1)	6
Chemical Physics Letters (2.3)	2
Molecular Physics (1.85)	30
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
Información Tecnológica	1
Anales de Física(0.3)	1
<b>Number of papers :</b>	<b>131</b>

Citations up to January 2009.

Total number of citations (ISI Web of knowledge) : 2302

Position in the world ranking of citations in Chemistry. Source : Web of knowledge. Area: Chemistry. Analyzed period 1997-2007. Date study : December 2008.

5558 by the number of citations.

3952 by the number of citations per paper.

**Factor H (h-index) = 26**

- 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 ).