

# **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).

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  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).

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  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*  
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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).

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  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).
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13. AUTHORS : C.Vega  
Title: *Perturbation theory of hard quadupolar fluids*  
Journal: Molec.Phys. **75**, 427–442, (1992)
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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).
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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).
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17. AUTHORS : C.Vega, E.P.A.Paras y P.A.Monson Title: *Solid-fluid equilibria for hard dumbbells via Monte Carlo simulation* Journal: J.Chem.Phys. **96**, 9060–9072, (1992).
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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)
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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).
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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).
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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).
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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).
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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).
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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).
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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).
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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).
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33. AUTHORS :P.Padilla y C.Vega Title: *Packing effects on the conformational equilibrium of alkanes* Journal:Molec.Phys. **84**, 435–450, (1995).
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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).
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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).
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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).
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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).
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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).
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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).
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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).
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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).
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64. AUTHORS :C.Vega Title: *Evaluating virial coefficients for multicomponent mixtures: hard sphere mixtures and flexible chains* Journal: *Molecular Physics* **98**, 973–985 , (2000).
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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).
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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).
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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).
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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).
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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).
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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).
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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).
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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).
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118. AUTHORS : C.Vega and E.G.Noya TITLE: *Revisiting the Frenkel-Ladd method to compute the free energy of solids: the Einstein molecule approach* JOURNAL: J.Chem.Phys. , **127**, 154113 , (2007).
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119. AUTHORS : E.G.Noya, C.Menduiña, J.L.Aragones y C.Vega TITLE: *Equation of state, thermal expansion coefficient and isothermal compressibility for ices I<sub>h</sub>, II, III, V and VI, as obtained from computer simulation* JOURNAL: J.Phys.Chem.B , **111**, 15877-15888 , (2007).
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120. AUTHORS : J.L.F.Abascal y C.Vega TITLE: *The water forcefield: importance of dipolar and quadrupolar interactions* JOURNAL: J.Phys.Chem.C , **111**, 15811-15822 , (2007).
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121. AUTHORS : J.L.F. Abascal, R. García Fernández, L.G. MacDowell, E. Sanz and C. Vega TITLE: *Ice: a fruitful source of information about liquid water* JOURNAL: J.Mol.Liq. , **136**, 214-220 , (2007).
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122. AUTHORS : J.B.Caballero, E.G.Noya y C.Vega TITLE: *Complete phase behaviour of the symmetrical colloidal electrolyte* JOURNAL: J.Chem.Phys. , **127**, 244910-1–244910-7 , (2007).
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123. AUTHORS (p.o. de firma): C.Vega, E.Sanz, J.L.F.Abascal and E.G.Noya TITLE: *Determination of phase diagrams via computer simulation: methodology and applications to water, electrolytes and proteins* JOURNAL: J.Phys.Condens.Matter **20**, 153101, (2008).
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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).
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125. AUTHORS (p.o. de firma): M.M.Conde, C.Vega y A.Patrykiewicz TITLE: *The thickness of a liquid layer on the free surface of ice as obtained from computer simulation.* JOURNAL: J.Chem.Phys. **129**,014702, (2008).
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126. AUTHORS (p.o. de firma): F. Gamez, S. Lago, B.Garzon, P.Merkling and C.Vega TITLE: *Vapor-liquid equilibrium of fluids composed by oblate molecules.* JOURNAL: Molecular Physics , **106**, 1331-1339, (2008).
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127. AUTHORS (p.o. de firma): E.G.Noya, M.M.Conde and C.Vega TITLE: *Computing the free energy of molecular solids by the Einstein molecule approach: Ices XIII and XIV and a simple model of proteins.* JOURNAL: J.Chem.Phys. , **129**, 104704-1, 104704-16, (2008).
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128. AUTHORS (p.o. de firma): C.Vega, J.L.F.Abascal, M.M.Conde and J.L.Aragones TITLE: *What ice can teach us about water interactions : a critical comparison of the performance of different water models* JOURNAL: Faraday Discussions , **141**, 251-276, (2009).
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129. AUTHORS (p.o. de firma): J.L.Aragones, M.M. Conde , E.G.Noya and C.Vega TITLE: *The phase diagram of water at high pressures as obtained by computer simulations of the TIP4P/2005 model: the appearance of a plastic crystal phase* JOURNAL: Phys.Chem.Chem.Phys. , **11**, 543-555, (2009).
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130. AUTHORS (p.o. de firma): J.L.F.Abascal, E.Sanz and C.Vega TITLE: *Triple points and coexistence properties of the dense phases of water calculated using computer simulation* JOURNAL: Phys.Chem.Chem.Phys. , **11**, 556-562 , (2009).
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131. 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).
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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).
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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).
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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).
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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) .
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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) .
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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).
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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).
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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).
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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).
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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).
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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).
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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).
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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).
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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).
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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).
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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).
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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).
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149. AUTHORS : J. L. Aragones , 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).
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150. AUTHORS : J. L. Aragones , 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).
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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).
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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).
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153. AUTHORS : J. L. Aragones , E. Sanz and C. Vega TITLE: *Solubility of NaCl in water by molecular simulation revisited* JOURNAL: Journal of Chemical Physics , 136, 244508 , (2012).
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154. AUTHORS : C.McBride , E.G. Noya , J.L. Aragones , M. M. Conde and C. Vega TITLE: *The phase diagram of water from quantum simulations* JOURNAL: Physical Chemistry Chemical Physics , 14, 10140 , (2012).
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155. AUTHORS : J. L. Aragones , 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).
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156. AUTHORS : C.McBride , J.L. Aragones , 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).
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157. AUTHORS : J. L. Aragones , 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).
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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).
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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).
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160. AUTHORS : C. Vega and S. Sokolowski TITLE: *Orest Pizio: scientist and friend Foreword* JOURNAL: CONDENSED MATTER PHYSICS , 15, 20101 , (2012).
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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).
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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).
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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).
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164. AUTHORS (p.o. de firma): J. B. Boreyko and B. R. Srkjanto and T. D. Nguyen and C. Vega and M. Fuentes-Cabrera and C. P. Collier TITLE : *Dynamic defrosting on nanostructured superhydrophobic surfaces* JOURNAL: *Langmuir* , 29, 9516 , (2013).
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165. AUTHORS (p.o. de firma): G. Jimenez-Serratos and A. Gil-Villegas and C. Vega and F. J. Blas TITLE : *Monte Carlo simulation of flexible trimers: From square well chains to amphiphilic primitive models* JOURNAL: *J. Chem. Phys.* , 139, 114901 , (2013).
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166. AUTHORS (p.o. de firma): J. R. Espinosa and E. Sanz and C. Valeriani and C. Vega TITLE : *On fluid-solid direct coexistence simulations: The pseudo-hard sphere model* JOURNAL: *J. Chem. Phys.* , 139, 144502 , (2013).
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167. AUTHORS (p.o. de firma): E. Sanz and C. Vega and J. R. Espinosa and R. Caballero-Bernal and J.L.F. Abascal and C.Valeriani TITLE : *Homogeneous Ice Nucleation at Moderate Supercooling from Molecular Simulation* JOURNAL: *J. Am. Chem. Soc.* , 135, 15008 , (2013).
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168. AUTHORS (p.o. de firma): M. M. Conde and M. A. Gonzalez and J. L. F. Abascal and C. Vega TITLE : *Determining the phase diagram of water from direct coexistence simulations: The phase diagram of the TIP4P/2005 model revisited* JOURNAL: *J. Chem. Phys.* , 139, 154505 , (2013).
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169. AUTHORS (p.o. de firma): J. L. Aragones and M. Rovere and C. Vega and P. Gallo TITLE : *Computer Simulation Study of the Structure of LiCl Aqueous Solutions: Test of Non Standard Mixing Rules in the Ion Interaction* JOURNAL: *J. Phys. Chem. B* , in press, (2014).
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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 : International 9th IUPAC Conference on Chemical Thermodynamic

Place : Lisbon, Portugal

DATE : July 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

Contribution : Poster

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

Place : Merseburg, Germany

DATE : August 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

Contribution : Invited Talk

CONGRESS : International. 10th IUPAC Conference on Chemical Thermodynamics

Place : Prague , Checoslovaquia

DATE : August 1988

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4. AUTHORS: C.Vega y D.Frenkel

Title: Monte Carlo study of rod like Kihara molecules

Contribution : Talk

CONGRESS : International. NATO ASI

PLACE: Bath, United Kingdom

DATE : September 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

Contribution : Poster

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

Place : Santiago de Compostela, Spain

DATE : September 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

Contribution : Poster

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

Place : Prague , Checoslovaquia

DATE : May 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

Contribution : Poster

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

Place : Lyon, France

DATE : July 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

Contribution : Poster

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

Place : Southampton, United Kingdom

DATE : December 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  
Contribution : Poster  
CONGRESS : International. 18th Statphys  
Place : Berlin, Germany  
DATE : August 1992

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10. AUTHORS: C.Vega  
Title: **Recent progress in understanding liquids**  
Contribution : **Invited lecture**  
Place : **Harvard Faculty Club, USA**  
DATE : **March 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**  
Contribution : **Oral communication**  
CONGRESS: *International. American Institute of Chemical Engineering Annual Meeting*  
Place : **MIAMI, FLORIDA , USA**  
Date : **1992**

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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 meeting of the Mexical Physical Society  
Place : Puebla, México  
DATE : October 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  
Contribution: Poster  
CONGRESS : Spanish Statistical Mechanics National meeting  
Place : El Escorial, Madrid  
DATE : May 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  
Contribution: Poster  
CONGRESS : International. Second liquid Matter Conference of the European Physical Society  
Place : Firenze , Italy  
DATE : September 1993

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15. AUTHORS: C.Vega  
Title: Vapor liquid equilibrium of dipolar linear Kihara fluids  
Contribution: Poster  
CONGRESS : International. IV Liblice Conference on the Statistical Mechanics of Liquids  
Place : Checoslovaquia  
DATE : June 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.  
Contribution: Invited talk.  
CONGRESS : International. Equilibrio de Fases (EQUIFASE).  
Place : Caracas, Venezuela  
DATE : June 1995

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17. AUTHORS: C.VEGA y P.A.MONSON  
Title: **EQUILIBRIO LÍQUIDO-SÓLIDO DE SISTEMAS MOLECULARES E IÓNICOS**  
Contribution: **Oral communication**  
CONGRESS: *National meeting of Statistical Mechanics*



Place : ZARAGOZA , Spain.  
AÑO: 1996

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18. AUTHORS: C.VEGA

Title: THE FLUID-SOLID EQUILIBRIUM OF IONIC SYSTEMS

Contribution: Oral communication

CONGRESS: *International. PRE-LIQUID MATTER CONFERENCE*

Place : University of 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

Contribution: Oral communication.

CONGRESS: *International. 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

Contribution : Invited talk.

CONGRESS :International. 10th Nordic Symposium on Computer Simulation

Place :Tallin, Estonia

DATE : July 1996

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

Title: UNDERSTANDING THE PHASE DIAGRAM OF QUADRUPOLAR FLUIDS

Contribution: Invited Conference

CONGRESS: *International. 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

Contribution: Poster

CONGRESS : National meeting on Statistical Mechanics

Place : Getafe, Spain

DATE : September 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

Contribution: Poster

CONGRESS : National meeting on the Liquid State.

Place : Aguadulce, Almería , Spain.

DATE : July 1998

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

Title: Vapor-Liquid equilibrium of linear and branched alkanes

Contribution: Poster

CONGRESS : International. European Molecular Liquids Conference

PLACE: Mureau, Austria

DATE : November 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

Contribution:Poster

CONGRESS : International. Thermodynamics 99

PLACE: London, United Kingdom.

DATE : March 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  
Contribution: Poster  
CONGRESS : International. IV Liquid Matter Conference of the European Physical Society PLACE:Granada, Spain.  
DATE : July 1999

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

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28. AUTHORS:C.Vega  
Title: Aplicaciones de la Mecánica Estadística al estudio de hidrocarburos  
Contribution: Invited talk.  
CONGRESS : Seminars on Statistical Mechanics of the University of Huelva.  
PLACE:Huelva, España  
DATE : May 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  
Contribution: Poster  
CONGRESS : National meeting on Statistical Mechanics.  
PLACE: Santiago de Compostela, Spain.  
DATE : September 2000

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30. AUTHORS: C.Menduiña, C.McBride y C.Vega  
Title: Second virial coefficient calculations of quadrupolar linear molecules and their mixtures  
Contribution: Poster  
CONGRESS : International. 16th IUPAC Conference on Chemical Thermodynamics  
PLACE:Halifax, Canada  
DATE : August 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  
Contribution: Oral communication  
CONGRESS : International. Thermodynamics 2001  
PLACE:Bristol, United Kingdom.  
DATE : April 2001.

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32. AUTHORS: C.Vega  
Title: **The effect of flexibility on the phase diagram of simple molecular models.**  
Contribution: **Invited talk.**  
CONGRESS : **Seminars of the Chemistry Department of the University of Durham.**  
PLACE: **University of Durham, United Kingdom.**  
DATE : **May 2001.**

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33. AUTHORS:C.Vega  
Title: **Simple models, complex fluids**  
Contribution: **Plenary invited talk.**  
CONGRESS : **International. Global Phase Diagrams, International Bunsen Conference**  
PLACE: **Koln, Germany**  
DATE : **August 2001**

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

CONGRESS : **International. 17th IUPAC Conference on Chemical Thermodynamics**

PLACE: **Rostock, Germany**

DATE : **August 2002**

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**35. AUTHORS: C.Vega**

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

Contribution: **Invited Talk**

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

PLACE: **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**

Contribution: **Talk**

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

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

DATE : **June , 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**

Contribution: **Talk**

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

PLACE: **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**

Contribution: **Poster**

CONGRESS : **International. SAFT Simposium.**

PLACE: **Barcelona.**

DATE : **December 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**

Contribution: **Talk**

CONGRESS : **International. Statphys 22.**

PLACE: **Bangalore, India.**

DATE : **5-9 July 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.**

Contribution: **Poster.**

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

PLACE: **Varanasi, India.**

DATE : **12-15 July 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**

Contribution: **Poster**

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

PLACE: **Genova, Italia.**

DATE : **29-31 August 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**

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

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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**  
Contribution: **Talk**  
CONGRESS : **Thermodynamics 2005 (organized by Royal Society of Chemistry)**  
PLACE: **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**  
Contribution: **Talk**  
CONGRESS : **6th Liquid Matter Conference (organized by the European Physical Society) , July 2005**  
PLACE: **Utrecht, Holanda**

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**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, June 2006**  
PLACE: **Lednice, Czech Republic**

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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**  
Contribution: **Talk**  
CONGRESS : **Cecam workshop. Patchy colloids, Proteins and Network forming liquids: Analogies and new insights from computer simulations , June 2006.**  
PLACE: **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**  
Contribution: **Poster**  
CONGRESS : **FOMMS (Foundations of Molecular Modeling and Simulation), July 2006**  
PLACE: **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**  
Contribution: **Talk**  
CONGRESS : **EMLG/JMLG Annual Meeting, Liquids systems under extreme conditions , September 2006**  
PLACE: **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**  
Contribution: **Plenary invited talk**  
CONGRESS : **CCP5 Annual meeting, September 2006.**  
PLACE: **Bradford, United Kingdom**

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**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 : **PPEPPD (Properties and Phase Equilibria for Product and Process Design) , May 2007.**  
Place: **Creta, Greece**

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**51. Authors : C. Vega**  
Title: **Water at interfaces interactions**  
Contribution : **Talk (**  
Congress: **Workshop on Theory and Computer Simulation of Inhomogeneous Fluids**  
Place : **Madrid**

Mes: May      Año: 2007

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- 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, September 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 , September 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 , September 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, Germany.**
- 
- 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, July 2008.**  
**Place: Lund, Suecia.**
- 
- 57. Authors: J.L. Aragonés, E.G. Noya, J.L.F. Abascal, M.M. Conde, C. Vega**  
**Title : Properties of ices at 0K A test of water models**  
**Contribution : Talk**  
**Congress: CCP5 (Collaborative Computational Project 5 - The Computer Simulation of Condensed Phase)**  
**Place : Sheffield (Reino Unido) July 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 , August 2008.**  
**Place: Edimburg, United Kingdom**
- 
- 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: **Prague, Czech Republic .**

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**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.**

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**62. AUTHORS: J. L. F. Abascal, M. M. Conde and J. L. Aragoes**

Title: **What ice can teach us about water interactions: a critical comparison of the performance of different water models**

Contribution: **Poster , Minneapolis, May 2009.**

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

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**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 September, 2009.**

Place: **Huelva , España.**

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**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 , September, 2009.**

Place: **London, United Kingdom.**

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**65. AUTHORS: C.Vega**

Title: **Can we describe water using computer simulations ?**

Contribution: **Invited Lecture (Physical Chemistry Department ).**

CONGRESS : **University of Oxford , May, 2010.**

Place: **Oxford, UK.**

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**66. AUTHORS: C.Vega**

Title: **Can we describe water using computer simulations ?**

Contribution: **Invited Lecture (Faculty of Physics ).**

CONGRESS : **University of Rome, La Sapienza, January 2010.**

Place: **Roma, Italia.**

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**67. AUTHORS: C.Vega**

Title: **Describing water using simple models.**

Contribution: **Invited Lecture (Faculty of Physics).**

CONGRESS : **University of Luxembourg , June 2010.**

Place: **Luxemburg**

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**68. AUTHORS: Carlos Vega.**

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

Contribution: **Talk.**

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

Place: **Lausanne, Switzerland.**

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**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.**

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**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** , July, 2011.

Place: **Lausanne, Switzerland.**

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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, September 2011**

Place: **Wien, Austria.**

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72. AUTHORS: **Carlos Vega .**

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

CONGRESS : **University of Freiburg**

Place: **Freiburg, Germany, March 2012.**

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73. AUTHORS: **Carlos Vega .**

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

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

Place: **Lviv, Ucraina.**

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74. AUTHORS: **Carlos Vega .**

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

CONGRESS : **Imperial College London, March 2013.**

Place: **London, United Kingdom.**

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75. AUTHORS: **Carlos Vega .**

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

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

Place: **Madison, USA.**

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76. AUTHORS: **Carlos Vega .**

Title: **The phase diagram of water as obtained from computer simulations** Contribution: **Invited talk.**

CONGRESS : **PPEPPD** , May 2013 .

Place: **Iguazu, Argentina.**

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

PhD student: **MARÍA MARTÍN CONDE**

University : **Universidad Complutense**

Faculty/School: **Ciencias Químicas**

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

PhD student : **JUAN LUIS ARAGONÉS GÓMEZ**

University : **Universidad Complutense**

Faculty/School : **Ciencias Químicas**



## VISITS TO OTHER LABS

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Institute : FOM  
Place : Amsterdam , Holland. Year :1987 Stay : 3 months.  
Host : Prof. Daan Frenkel. Computer simulations of linear molecules.

Institute : Institute of Fluids and Thermodynamics . University of Bochum.  
Place : Bochum , Germany. Year :1989 Stay : 3 months.  
Host : Prof. Johan Fischer. Molecular Dynamics of the refrigerant R152a.

Institute : Department of Chemical Engineering . University of Cornell.  
Place : Ithaca , University of Cornell, USA. Year :1990 Stay : 2 months.  
Host : Prof. Keith Gubbins. Computer simulations of polar fluids.

Institute : Department of Chemical Engineering. University of Massachusetts.  
Place : Amherst , U. Massachusetts, USA. Year :1991-1992 Stay : 16 months.  
Host : Prof. Peter Monson, Phase diagram of diatomic molecules via computer simulations.

Institute : Department of Chemical Engineering. University of Massachusetts.  
Place : Amherst , U. Massachusetts, USA. Year : 1997 Stay : 2 months.  
Host : Prof. Peter Monson, Phase diagram of molecules with hydrogen bonds. NATO COLABORATIVE GRANT

Institute : Faculty of Chemistry. University Marie Curie Skolowska.  
Place : Lublin , Poland. Year : 2006. Stay : 2 months.  
Host : Prof. A. Patrykiewicz and Prof. S. Sokolowski. Computer simulation study of the ice-vapor interface. European Project MTKD-CT-2004-509249.

## Publications analysis.

Journal (impact factor)	Number
Physical Review Letters(6)	4
Journal of the American Chemical Society(10)	1
Faraday Discussion (5)	1
Langmuir (4.5)	2
Journal of Chemical Physics (3.3)	80
Journal of Physical Chemistry (4)	6
Journal of Physical Chemistry B (3.6)	6
Journal of Physical Chemistry C (2)	2
Journal of Physical Chemistry A (2.5)	1
Physical Chemistry and Chemical Physics (3.5)	12
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 :	167

Citation analysis, updated , April , 2014.

Total number of citations : 5112

Papers with more than 100 citations : 9

**H (h-index) = 38**

Algorithm search for ISI :

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 Faculty of Chemistry in Complutense University.
- Since January 2007 I belong to the Advisory Editorial Board of Molecular Physics.
- Since January 2014 I belong to the Advisory Editorial Board of the Journal of Chemical Physics.
- I act as referee for the following journals (8-10 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 to work with Prof. Peter A. Monson .

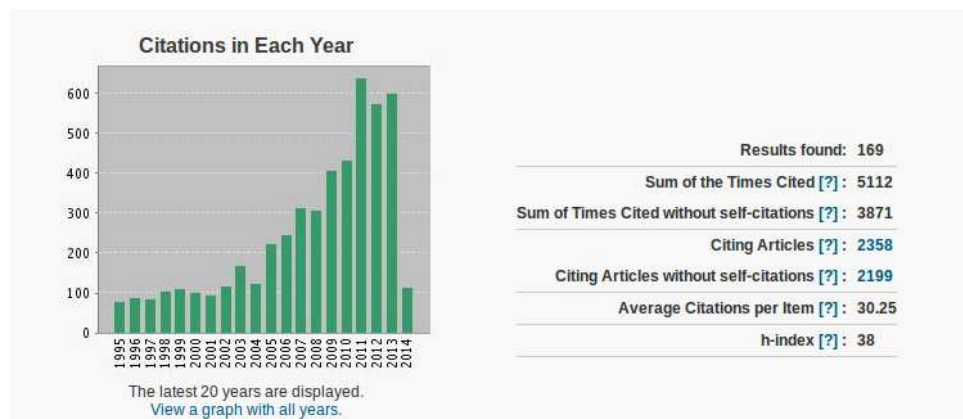


Figura 1: History of papers and citations according to ISI ( Research ID : C-5455-2009 )

Web page of the group: [catalan.quim.ucm.es](http://catalan.quim.ucm.es)