Carlos Vega

List of Publications by Year
in descending order

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225 papers	16,941 citations	23879 60 h-index	18944 123 g-index
229 all docs	229 docs citations	229 times ranked	9363 citing authors

#	Article	IF	Citations
1	On the thermodynamics of curved interfaces and the nucleation of hard spheres in a finite system. Journal of Chemical Physics, 2022, 156, 014505.	1.2	4
2	The Madrid-2019 force field for electrolytes in water using TIP4P/2005 and scaled charges: Extension to the ions Fâ˜, Brâ˜, Iâ˜, Rb+, and Cs+. Journal of Chemical Physics, 2022, 156, 044505.	1.2	36
3	Freezing point depression of salt aqueous solutions using the Madrid-2019 model. Journal of Chemical Physics, 2022, 156, 134503.	1.2	21
4	Maximum in density of electrolyte solutions: Learning about ionâ€“water interactions and testing the Madrid-2019 force field. Journal of Chemical Physics, 2022, 156, 154502.	1.2	13
5	Melting points of water models: Current situation. Journal of Chemical Physics, 2022, 156, .	1.2	14
6	Parasitic crystallization of colloidal electrolytes: growing a metastable crystal from the nucleus of a stable phase. Soft Matter, 2021, 17, 489-505.	1.2	11
7	Fcc vs. hcp competition in colloidal hard-sphere nucleation: on their relative stability, interfacial free energy and nucleation rate. Physical Chemistry Chemical Physics, 2021, 23, 19611-19626.	1.3	18
8	Anomalous Behavior in the Nucleation of Ice at Negative Pressures. Physical Review Letters, 2021, 126, 015704.	2.9	24
9	â€œIn Silicoâ€•Seawater. Journal of Chemical Theory and Computation, 2021, 17, 1715-1725.	2.3	20
10	Homogeneous nucleation of NaCl in supersaturated solutions. Physical Chemistry Chemical Physics, 2021, 23, 26843-26852.	1.3	20
11	2020 JCP Emerging Investigator Special Collection. Journal of Chemical Physics, 2021, 155, 230401.	1.2	1
12	JCP Emerging Investigator Special Collection 2019. Journal of Chemical Physics, 2020, 153, 110402.	1.2	2
13	The Youngâ€“Laplace equation for a solidâ€“liquid interface. Journal of Chemical Physics, 2020, 153, 191102.	1.2	35
14	Antifreeze proteins and homogeneous nucleation: On the physical determinants impeding ice crystal growth. Journal of Chemical Physics, 2020, 153, 091102.	1.2	7
15	Scaled charges at work: Salting out and interfacial tension of methane with electrolyte solutions from computer simulations. Fluid Phase Equilibria, 2020, 513, 112548.	1.4	33
16	Interfacial Free Energy and Tolman Length of Curved Liquidâ€“Solid Interfaces from Equilibrium Studies. Journal of Physical Chemistry C, 2020, 124, 8795-8805.	1.5	24
17	Seeding approach to nucleation in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>N</mml:mi><mml:mi>V</mml:mi><mml:mi>T</mml:mi> ensemble: The case of bubble cavitation in overstretched Lennard Jones fluids. Physical Review E, 2020, 101, 022611.	0.8	28
18	Equivalence between condensation and boiling in a Lennard-Jones fluid. Physical Review E, 2020, 102, 062609.	0.8	14

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19	Ice growth rate: Temperature dependence and effect of heat dissipation. Journal of Chemical Physics, 2019, 151, 044509.	1.2	20
20	Interfacial free energy of a liquid-solid interface: Its change with curvature. Journal of Chemical Physics, 2019, 151, 144501.	1.2	28
21	A force field of Li+, Na+, K+, Mg2+, Ca2+, Clâ˜, and SO42â˜ in aqueous solution based on the TIP4P/2005 water model and scaled charges for the ions. Journal of Chemical Physics, 2019, 151, 134504.	1.2	166
22	Nucleation of pseudo hard-spheres and dumbbells at moderate metastability: appearance of A15 Frankâ€“Kasper phase at intermediate elongations. Physical Chemistry Chemical Physics, 2019, 21, 1656-1670.	1.3	5
23	Breakdown of the law of rectilinear diameter and related surprises in the liquid-vapor coexistence in systems of patchy particles. Journal of Chemical Physics, 2019, 150, 224510.	1.2	30
24	Ice Ih vs. ice III along the homogeneous nucleation line. Physical Chemistry Chemical Physics, 2019, 21, 5655-5660.	1.3	10
25	Seeding approach to bubble nucleation in superheated Lennard-Jones fluids. Physical Review E, 2019, 100, 052609.	0.8	9
26	Heterogeneous versus homogeneous crystal nucleation of hard spheres. Soft Matter, 2019, 15, 9625-9631.	1.2	27
27	A simulation study of homogeneous ice nucleation in supercooled salty water. Journal of Chemical Physics, 2018, 148, 222811.	1.2	33
28	Phase boundaries, nucleation rates and speed of crystal growth of the water-to-ice transition under an electric field: a simulation study. Journal of Physics Condensed Matter, 2018, 30, 174002.	0.7	12
29	Calculation of the water-octanol partition coefficient of cholesterol for SPC, TIP3P, and TIP4P water. Journal of Chemical Physics, 2018, 149, 224501.	1.2	12
30	Homogeneous Ice Nucleation Rate in Water Droplets. Journal of Physical Chemistry C, 2018, 122, 22892-22896.	1.5	25
31	NaCl nucleation from brine in seeded simulations: Sources of uncertainty in rate estimates. Journal of Chemical Physics, 2018, 148, 222838.	1.2	62
32	Continuous version of a square-well potential of variable range and its application in molecular dynamics simulations. Molecular Physics, 2018, 116, 3355-3365.	0.8	11
33	Estimating the solubility of 1:1 electrolyte aqueous solutions: the chemical potential difference rule. Molecular Physics, 2017, 115, 1301-1308.	0.8	21
34	Special Issue of Molecular Physics in Honour of Professor Johann Fischer. Molecular Physics, 2017, 115, 1015-1016.	0.8	0
35	A potential model for sodium chloride solutions based on the TIP4P/2005 water model. Journal of Chemical Physics, 2017, 147, 104501.	1.2	82
36	Role of Salt, Pressure, and Water Activity on Homogeneous Ice Nucleation. Journal of Physical Chemistry Letters, 2017, 8, 4486-4491.	2.1	33

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37	Water: A Tale of Two Liquids. Chemical Reviews, 2016, 116, 7463-7500.	23.0	627
38	On the calculation of solubilities via direct coexistence simulations: Investigation of NaCl aqueous solutions and Lennard-Jones binary mixtures. Journal of Chemical Physics, 2016, 145, 154111.	1.2	80
39	Editorial: The Future of Chemical Physics Conference 2016. Journal of Chemical Physics, 2016, 145, 220401.	1.2	1
40	On the time required to freeze water. Journal of Chemical Physics, 2016, 145, 211922.	1.2	64
41	Seeding approach to crystal nucleation. Journal of Chemical Physics, 2016, 144, 034501.	1.2	155
42	Consensus on the solubility of NaCl in water from computer simulations using the chemical potential route. Journal of Chemical Physics, 2016, 144, 124504.	1.2	108
43	A new intermolecular potential for simulations of methanol: The OPLS/2016 model. Journal of Chemical Physics, 2016, 145, 034508.	1.2	30
44	Iceâ€“Water Interfacial Free Energy for the TIP4P, TIP4P/2005, TIP4P/Ice, and mW Models As Obtained from the Mold Integration Technique. Journal of Physical Chemistry C, 2016, 120, 8068-8075.	1.5	79
45	Interfacial Free Energy as the Key to the Pressure-Induced Deceleration of Ice Nucleation. Physical Review Letters, 2016, 117, 135702.	2.9	65
46	Lattice mold technique for the calculation of crystal nucleation rates. Faraday Discussions, 2016, 195, 569-582.	1.6	4
47	Competition between ices Ih and Ic in homogeneous water freezing. Journal of Chemical Physics, 2015, 143, 134504.	1.2	65
48	The A in SAFT: developing the contribution of association to the Helmholtz free energy within a Wertheim TPT1 treatment of generic Mie fluids. Molecular Physics, 2015, 113, 948-984.	0.8	114
49	Water: one molecule, two surfaces, one mistake. Molecular Physics, 2015, 113, 1145-1163.	0.8	51
50	Reminiscences about TomÃ¡Å¡ BoublÃk, Ivo Nezbeda and the Liblice Meetings on the Statistical Mechanics of Liquids. Molecular Physics, 2015, 113, 891-897.	0.8	0
51	Molecular dynamics simulation of CO2 hydrates: Prediction of three phase coexistence line. Journal of Chemical Physics, 2015, 142, 124505.	1.2	96
52	The crystal-fluid interfacial free energy and nucleation rate of NaCl from different simulation methods. Journal of Chemical Physics, 2015, 142, 194709.	1.2	59
53	Homogeneous ice nucleation evaluated for several water models. Journal of Chemical Physics, 2014, 141, 18C529.	1.2	128
54	The mold integration method for the calculation of the crystal-fluid interfacial free energy from simulations. Journal of Chemical Physics, 2014, 141, 134709.	1.2	58

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55	Nucleation free-energy barriers with Hybrid Monte-Carlo/Umbrella Sampling. Physical Chemistry Chemical Physics, 2014, 16, 24913-24919.	1.3	13
56	Computer Simulation Study of the Structure of LiCl Aqueous Solutions: Test of Non-Standard Mixing Rules in the Ion Interaction. Journal of Physical Chemistry B, 2014, 118, 7680-7691.	1.2	36
57	Free energy calculations for molecular solids using <scp>GROMACS</scp>. Journal of Chemical Physics, 2013, 139, 034104.	1.2	46
58	Dynamic Defrosting on Nanostructured Superhydrophobic Surfaces. Langmuir, 2013, 29, 9516-9524.	1.6	158
59	On fluid-solid direct coexistence simulations: The pseudo-hard sphere model. Journal of Chemical Physics, 2013, 139, 144502.	1.2	92
60	Monte Carlo simulation of flexible trimers: From square well chains to amphiphilic primitive models. Journal of Chemical Physics, 2013, 139, 114901.	1.2	9
61	Homogeneous Ice Nucleation at Moderate Supercooling from Molecular Simulation. Journal of the American Chemical Society, 2013, 135, 15008-15017.	6.6	256
62	A computer program to evaluate the NVM propagator for rigid asymmetric tops for use in path integral simulations of rigid bodies. Computer Physics Communications, 2013, 184, 885-890.	3.0	6
63	Note: A simple correlation to locate the three phase coexistence line in methane-hydrate simulations. Journal of Chemical Physics, 2013, 138, 056101.	1.2	54
64	Determining the phase diagram of water from direct coexistence simulations: The phase diagram of the TIP4P/2005 model revisited. Journal of Chemical Physics, 2013, 139, 154505.	1.2	61
65	Fluid-solid equilibrium of carbon dioxide as obtained from computer simulations of several popular potential models: The role of the quadrupole. Journal of Chemical Physics, 2013, 138, 084506.	1.2	21
66	Local order parameters for use in driving homogeneous ice nucleation with all-atom models of water. Journal of Chemical Physics, 2012, 137, 194504.	1.2	98
67	Note: Free energy calculations for atomic solids through the Einstein crystal/molecule methodology using GROMACS and LAMMPS. Journal of Chemical Physics, 2012, 137, 146101.	1.2	37
68	A study of the influence of isotopic substitution on the melting point and temperature of maximum density of water by means of path integral simulations of rigid models. Physical Chemistry Chemical Physics, 2012, 14, 15199.	1.3	20
69	The phase diagram of water from quantum simulations. Physical Chemistry Chemical Physics, 2012, 14, 10140.	1.3	36
70	Calculation of the melting point of alkali halides by means of computer simulations. Journal of Chemical Physics, 2012, 137, 104507.	1.2	41
71	Solubility of NaCl in water by molecular simulation revisited. Journal of Chemical Physics, 2012, 136, 244508.	1.2	133
72	Evaluation of the pressure tensor and surface tension for molecular fluids with discontinuous potentials using the volume perturbation method. Journal of Chemical Physics, 2012, 137, 204104.	1.2	18

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73	Freezing Transition and Interaction Potential in Monolayers of Microparticles at Fluid Interfaces. Langmuir, 2011, 27, 3391-3400.	1.6	51
74	Dielectric Constant of Ices and Water: A Lesson about Water Interactions. Journal of Physical Chemistry A, 2011, 115, 5745-5758.	1.1	108
75	Solidâ^'Solid and Solidâ^'Fluid Equilibria of the Most Popular Models of Methanol Obtained by Computer Simulation. Journal of Physical Chemistry B, 2011, 115, 3522-3530.	1.2	9
76	Note: Equation of state and compressibility of supercooled water: Simulations and experiment. Journal of Chemical Physics, 2011, 134, 186101.	1.2	52
77	Physics and chemistry of water and ice. Physical Chemistry Chemical Physics, 2011, 13, 19660.	1.3	12
78	Simulating water with rigid non-polarizable models: a general perspective. Physical Chemistry Chemical Physics, 2011, 13, 19663.	1.3	749
79	Phase Diagram of Water under an Applied Electric Field. Physical Review Letters, 2011, 107, 155702.	2.9	53
80	Path integral Monte Carlo simulations for rigid rotors and their application to water. Molecular Physics, 2011, 109, 149-168.	0.8	25
81	A quantum propagator for path-integral simulations of rigid molecules. Journal of Chemical Physics, 2011, 134, 054117.	1.2	17
82	The stability of a crystal with diamond structure for patchy particles with tetrahedral symmetry. Journal of Chemical Physics, 2010, 132, 234511.	1.2	93
83	Dielectric Constant of Ice Ih and Ice V: A Computer Simulation Study. Journal of Physical Chemistry B, 2010, 114, 6089-6098.	1.2	31
84	Nuclear Quantum Effects in Water Clusters: The Role of the Molecular Flexibility. Journal of Physical Chemistry B, 2010, 114, 2484-2492.	1.2	30
85	Widom line and the liquidâ€"liquid critical point for the TIP4P/2005 water model. Journal of Chemical Physics, 2010, 133, 234502.	1.2	267
86	Heat capacity of water: A signature of nuclear quantum effects. Journal of Chemical Physics, 2010, 132, 046101.	1.2	90
87	Determining the three-phase coexistence line in methane hydrates using computer simulations. Journal of Chemical Physics, 2010, 133, 064507.	1.2	201
88	Melting point and phase diagram of methanol as obtained from computer simulations of the OPLS model. Journal of Chemical Physics, 2010, 132, 094505.	1.2	20
89	Can gas hydrate structures be described using classical simulations?. Journal of Chemical Physics, 2010, 132, 114503.	1.2	44
90	Quantum contributions in the ice phases: The path to a new empirical model for waterâ€"TIP4PQ/2005. Journal of Chemical Physics, 2009, 131, 024506.	1.2	62

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91	Quantum effects on the maximum in density of water as described by the TIP4PQ/2005 model. Journal of Chemical Physics, 2009, 131, 124518.	1.2	26
92	Anomalies in water as obtained from computer simulations of the TIP4P/2005 model: density maxima, and density, isothermal compressibility and heat capacity minima. Molecular Physics, 2009, 107, 365-374.	0.8	153
93	Plastic crystal phases of simple water models. Journal of Chemical Physics, 2009, 130, 244504.	1.2	65
94	The phase diagram of water at high pressures as obtained by computer simulations of the TIP4P/2005 model: the appearance of a plastic crystal phase. Physical Chemistry Chemical Physics, 2009, 11, 543-555.	1.3	72
95	Triple points and coexistence properties of the dense phases of water calculated using computer simulation. Physical Chemistry Chemical Physics, 2009, 11, 556-562.	1.3	26
96	What ice can teach us about water interactions: a critical comparison of the performance of different water models. Faraday Discussions, 2009, 141, 251-276.	1.6	375
97	The phase diagram of water at negative pressures: Virtual ices. Journal of Chemical Physics, 2009, 131, 034510.	1.2	69
98	Determination of phase diagrams via computer simulation: methodology and applications to water, electrolytes and proteins. Journal of Physics Condensed Matter, 2008, 20, 153101.	0.7	209
99	Vapourâ€“liquid equilibrium of fluids composed by oblate molecules. Molecular Physics, 2008, 106, 1331-1339.	0.8	14
100	Computing the free energy of molecular solids by the Einstein molecule approach: Ices XIII and XIV, hard-dumbbells and a patchy model of proteins. Journal of Chemical Physics, 2008, 129, 104704.	1.2	58
101	Determination of the melting point of hard spheres from direct coexistence simulation methods. Journal of Chemical Physics, 2008, 128, 154507.	1.2	97
102	The thickness of a liquid layer on the free surface of ice as obtained from computer simulation. Journal of Chemical Physics, 2008, 129, 014702.	1.2	142
103	Phase diagram of model anisotropic particles with octahedral symmetry. Journal of Chemical Physics, 2007, 127, 054501.	1.2	80
104	Solubility of KF and NaCl in water by molecular simulation. Journal of Chemical Physics, 2007, 126, 014507.	1.2	107
105	Complete phase behavior of the symmetrical colloidal electrolyte. Journal of Chemical Physics, 2007, 127, 244910.	1.2	9
106	Surface tension of the most popular models of water by using the test-area simulation method. Journal of Chemical Physics, 2007, 126, 154707.	1.2	635
107	Dipole-Quadrupole Force Ratios Determine the Ability of Potential Models to Describe the Phase Diagram of Water. Physical Review Letters, 2007, 98, 237801.	2.9	69
108	Properties of ices at 0 K: A test of water models. Journal of Chemical Physics, 2007, 127, 154518.	1.2	32

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109	The Water Forcefield:â€‰Importance of Dipolar and Quadrupolar Interactions. Journal of Physical Chemistry C, 2007, 111, 15811-15822.	1.5	54
110	The melting point of hexagonal ice (Ih) is strongly dependent on the quadrupole of the water models. Physical Chemistry Chemical Physics, 2007, 9, 2775.	1.3	30
111	Equation of State, Thermal Expansion Coefficient, and Isothermal Compressibility for Ices Ih, II, III, V, and VI, as Obtained from Computer Simulationâ€. Journal of Physical Chemistry C, 2007, 111, 15877-15888.	1.5	39
112	Investigation of the Salting Out of Methane from Aqueous Electrolyte Solutions Using Computer Simulations. Journal of Physical Chemistry B, 2007, 111, 8993-9000.	1.2	36
113	Revisiting the Frenkel-Ladd method to compute the free energy of solids: The Einstein molecule approach. Journal of Chemical Physics, 2007, 127, 154113.	1.2	139
114	Ice: A fruitful source of information about liquid water. Journal of Molecular Liquids, 2007, 136, 214-220.	2.3	15
115	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 of Chemical Physics, 2006, 125, 034503.	1.2	210
116	The melting temperature of the six site potential model of water. Journal of Chemical Physics, 2006, 125, 166101.	1.2	74
117	The melting point of ice Ih for common water models calculated from direct coexistence of the solid-liquid interface. Journal of Chemical Physics, 2006, 124, 144506.	1.2	386
118	Absence of superheating for icelhwith a free surface: a new method of determining the melting point of different water models. Molecular Physics, 2006, 104, 3583-3592.	0.8	63
119	Computer simulation of two new solid phases of water: Ice XIII and ice XIV. Journal of Chemical Physics, 2006, 125, 116101.	1.2	15
120	A potential model for methane in water describing correctly the solubility of the gas and the properties of the methane hydrate. Journal of Chemical Physics, 2006, 125, 074510.	1.2	139
121	Non-Markovian melting: a novel procedure to generate initial liquid like phases for small molecules for use in computer simulation studies. Computer Physics Communications, 2005, 170, 137-143.	3.0	1
122	Radial distribution functions and densities for the SPC/E, TIP4P and TIP5P models for liquid water and ices Ih, Ic, II, III, IV, V, VI, VII, VIII, IX, XI and XII. Physical Chemistry Chemical Physics, 2005, 7, 1450.	1.3	111
123	Relation between the melting temperature and the temperature of maximum density for the most common models of water. Journal of Chemical Physics, 2005, 123, 144504.	1.2	117
124	Can simple models describe the phase diagram of water?. Journal of Physics Condensed Matter, 2005, 17, S3283-S3288.	0.7	72
125	The range of meta stability of ice-water melting for two simple models of water. Molecular Physics, 2005, 103, 1-5.	0.8	54
126	A potential model for the study of ices and amorphous water: TIP4P/Ice. Journal of Chemical Physics, 2005, 122, 234511.	1.2	1,041

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127	The melting temperature of the most common models of water. Journal of Chemical Physics, 2005, 122, 114507.	1.2	338
128	A general purpose model for the condensed phases of water: TIP4P/2005. Journal of Chemical Physics, 2005, 123, 234505.	1.2	2,907
129	Tracing the phase diagram of the four-site water potential (TIP4P). Journal of Chemical Physics, 2004, 121, 1165-1166.	1.2	73
130	Combinatorial entropy and phase diagram of partially ordered ice phases. Journal of Chemical Physics, 2004, 121, 10145-10158.	1.2	54
131	Formation of high density amorphous ice by decompression of ice VII and ice VIII at 135 K. Journal of Chemical Physics, 2004, 121, 11907-11911.	1.2	24
132	Molecular modeling of flexible molecules. Vaporâ€“liquid and fluidâ€“solid equilibria. Journal of Molecular Liquids, 2004, 113, 37-51.	2.3	12
133	Computer simulation study of the global phase behavior of linear rigid Lennard-Jones chain molecules: Comparison with flexible models. Journal of Chemical Physics, 2004, 120, 3957-3968.	1.2	27
134	Phase Diagram of Water from Computer Simulation. Physical Review Letters, 2004, 92, 255701.	2.9	264
135	The properties of fully flexible Lennard-Jones chains in the solid phase: Wertheim theory and simulation. Molecular Physics, 2003, 101, 2241-2255.	0.8	17
136	Fluidâ€“solid equilibria of flexible and linear rigid tangent chains from Wertheimâ€™s thermodynamic perturbation theory. Journal of Chemical Physics, 2003, 119, 10958-10971.	1.2	17
137	The fluidâ€“solid equilibrium for a charged hard sphere model revisited. Journal of Chemical Physics, 2003, 119, 964-971.	1.2	59
138	Third virial coefficients and critical properties of quadrupolar two center Lennard-Jones models. Physical Chemistry Chemical Physics, 2003, 5, 2851-2857.	1.3	18
139	The phase diagram of the two center Lennard-Jones model as obtained from computer simulation and Wertheimâ€™s thermodynamic perturbation theory. Journal of Chemical Physics, 2003, 118, 10696-10706.	1.2	33
140	Critical properties of molecular fluids from the virial series. Journal of Chemical Physics, 2003, 119, 11367-11373.	1.2	18
141	Characterization of the order-disorder transition of a charged hard-sphere model. Physical Review E, 2003, 68, 052501.	0.8	8
142	Bonded hard-sphere theory and computer simulation of the equation of state of linear fusedâ€“hard-sphere fluids. Journal of Chemical Physics, 2003, 119, 9633-9639.	1.2	9
143	Study of the solid-liquid-vapour phase equilibria of flexible chain molecules using Wertheim's thermodynamic perturbation theory. Molecular Physics, 2003, 101, 449-458.	0.8	27
144	Scaling laws for the equation of state of flexible and linear tangent hard sphere chains. Physical Review E, 2002, 65, 052501.	0.8	9

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145	Extending Wertheimâ€™s perturbation theory to the solid phase of Lennard-Jones chains: Determination of the global phase diagram. Journal of Chemical Physics, 2002, 116, 7645-7655.	1.2	35
146	Fluid solid equilibrium for two dimensional tangent hard disk chains from Wertheimâ€™s perturbation theory. Journal of Chemical Physics, 2002, 116, 1757-1759.	1.2	22
147	The global phase diagram of the Gayâ€“Berne model. Journal of Chemical Physics, 2002, 117, 6313-6322.	1.2	82
148	A computer simulation study of racemic mixtures. Molecular Physics, 2002, 100, 2397-2415.	0.8	11
149	The second virial coefficient of the dipolar two center Lennard-Jones modelElectronic supplementary information (ESI) available: computer programs and ancillary data. See http://www.rsc.org/suppdata/cp/b2/b200781a/. Physical Chemistry Chemical Physics, 2002, 4, 3000-3007.	1.3	30
150	The effect of flexibility on the phase diagram of simple molecular models. Physical Chemistry Chemical Physics, 2002, 4, 853-862.	1.3	18
151	A Monte Carlo study of the influence of molecular flexibility on the phase diagram of a fused hard sphere model. Journal of Chemical Physics, 2002, 117, 10370-10379.	1.2	35
152	Equation of state of model branched alkanes: Theoretical predictions and configurational bias Monte Carlo simulations. Journal of Chemical Physics, 2001, 115, 6220-6235.	1.2	15
153	The second virial coefficient of quadrupolar two center Lennard-Jones models. Physical Chemistry Chemical Physics, 2001, 3, 1289-1296.	1.3	24
154	Isotropic-nematic phase transition: Influence of intramolecular flexibility using a fused hard sphere model. Physical Review E, 2001, 64, 011703.	0.8	46
155	Extending Wertheimâ€™s perturbation theory to the solid phase: The freezing of the pearl-necklace model. Journal of Chemical Physics, 2001, 114, 10411-10418.	1.2	48
156	Liquid crystal phase formation for the linear tangent hard sphere model from Monte Carlo simulations. Journal of Chemical Physics, 2001, 115, 4203-4211.	1.2	53
157	Evaluating virial coefficients for multicomponent mixtures: hard sphere mixtures and flexible chains. Molecular Physics, 2000, 98, 973-985.	0.8	16
158	Critical temperature of infinitely long chains from Wertheim's perturbation theory. Molecular Physics, 2000, 98, 1295-1308.	0.8	29
159	The virial coefficients of the pearl-necklace model. Journal of Chemical Physics, 2000, 113, 10398-10409.	1.2	24
160	Order-Disorder Transition in the Solid Phase of a Charged Hard Sphere Model. Physical Review Letters, 2000, 85, 3217-3220.	2.9	49
161	Equation of state and critical behavior of polymer models: A quantitative comparison between Wertheimâ€™s thermodynamic perturbation theory and computer simulations. Journal of Chemical Physics, 2000, 113, 419-433.	1.2	76
162	An application of cell theory to molecular models of n-alkane solids. Molecular Physics, 2000, 98, 363-370.	0.8	8

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163	Excess properties of mixtures of n-alkanes from perturbation theory. Journal of Chemical Physics, 1999, 111, 3192-3202.	1.2	9
164	Determination of potential parameters for alkanes. Journal of Chemical Physics, 1999, 111, 438-439.	1.2	13
165	Critical properties of mixtures of alkanes from perturbation theory. Journal of Chemical Physics, 1999, 111, 3183-3191.	1.2	9
166	Monte Carlo simulations of dipolar and quadrupolar linear Kihara fluids. A test of thermodynamic perturbation theory. Molecular Physics, 1999, 96, 123-132.	0.8	10
167	Understanding the phase diagrams of quadrupolar molecules. Journal of Molecular Liquids, 1998, 76, 157-169.	2.3	9
168	Vaporâ€“liquid equilibria of linear and branched alkanes from perturbation theory. Journal of Chemical Physics, 1998, 109, 5681-5690.	1.2	15
169	Adsorption of Dimerizing and Dimer Fluids in Disordered Porous Media. Journal of Physical Chemistry B, 1998, 102, 3012-3017.	1.2	18
170	Solidâ€“fluid equilibrium for a molecular model with short ranged directional forces. Journal of Chemical Physics, 1998, 109, 9938-9949.	1.2	68
171	Structure and phase diagram of mixtures of hard spheres in the limit of infinite size ratio. Journal of Chemical Physics, 1998, 108, 3074-3075.	1.2	15
172	The second virial coefficient of hard alkane models. Journal of Chemical Physics, 1998, 109, 5670-5680.	1.2	21
173	The structure and adsorption of diatomic fluids in disordered porous media. A Monte Carlo simulation study. Molecular Physics, 1998, 95, 701-712.	0.8	2
174	Adsorption isotherm for flexible molecules in random porous media. Can we regard the system as a binary mixture?. Journal of Chemical Physics, 1997, 106, 1997-2011.	1.2	20
175	Accurate Simulations of the Vaporâ^'Liquid Equilibrium of Important Organic Solvents and Other Diatomics. Journal of Physical Chemistry B, 1997, 101, 6763-6771.	1.2	28
176	Plastic crystal phases of hard dumbbells and hard spherocylinders. Journal of Chemical Physics, 1997, 107, 2696-2697.	1.2	58
177	Solid-fluid equilibrium: new perspectives from molecular theory. Fluid Phase Equilibria, 1996, 117, 114-125.	1.4	15
178	Absence of criticality in the reference hypernetted chain equation for short ranged potentials. Molecular Physics, 1996, 87, 1235-1242.	0.8	5
179	Fluid-solid equilibrium of a charged hard-sphere model. Physical Review E, 1996, 54, 2746-2760.	0.8	48
180	Equation of state for hardnâ€alkane models: Long chains. Journal of Chemical Physics, 1996, 104, 701-713.	1.2	30

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181	Second virial coefficients, critical temperatures, and the molecular shapes of long nâ€alkanes. Journal of Chemical Physics, 1996, 105, 4223-4233.	1.2	23
182	Thermodynamics of fluids obtained by mapping the collision properties. Physical Review E, 1996, 53, 2326-2336.	0.8	25
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