

# Ariel A Chialvo

## List of Publications by Year in descending order

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docs citations

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times ranked

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#	ARTICLE	IF	CITATIONS
1	On density-based modeling of dilute non-electrolyte solutions involving wide ranges of state conditions and intermolecular asymmetries: Formal results, fundamental constraints, and the rationale for its molecular thermodynamic foundations. <i>Fluid Phase Equilibria</i> , 2021, 535, 112969.	1.4	7
2	Osmolyte-Induced Effects on the Hydration Behavior and the Osmotic Second Virial Coefficients of Alkyl-Substituted Urea Derivatives: Critical Assessment of Their Structure-Making/Breaking Behavior. <i>Journal of Physical Chemistry B</i> , 2021, 125, 6231-6243.	1.2	6
3	Can Jones's "Dole's" B-Coefficient be a Consistent Structure-Making/Breaking Marker? Rigorous Molecular-Based Analysis and Critical Assessment of Its Marker Uniqueness. <i>Journal of Physical Chemistry B</i> , 2021, 125, 12028-12041.	1.2	11
4	On the linear orthobaric-density representation of near-critical solvation quantities: What can we conclude about the accuracy of this paradigm?. <i>Fluid Phase Equilibria</i> , 2020, 514, 112535.	1.4	9
5	On the Solvation Thermodynamics Involving Species with Large Intermolecular Asymmetries: A Rigorous Molecular-Based Approach to Simple Systems with Unconventionally Complex Behaviors. <i>Journal of Physical Chemistry B</i> , 2020, 124, 7879-7896.	1.2	12
6	On the Krichevskii parameter of solutes in dilute solutions: Formal links between its magnitude, the solute-solvent intermolecular asymmetry, and the precise description of solution thermodynamics. <i>Fluid Phase Equilibria</i> , 2020, 513, 112546.	1.4	10
7	Behaviour of rarified steam at very high temperature an orientation-averaged interaction potential approach towards its accurate description. <i>Molecular Physics</i> , 2019, 117, 3922-3940.	0.8	3
8	Solute-induced effects in solvation thermodynamics: does urea behave as a structure-making or structure-breaking solute?. <i>Molecular Physics</i> , 2019, 117, 3484-3492.	0.8	12
9	Solvation behavior of solutes in dilute solutions novel formal results, rules of thumb, and potential modeling pitfalls. <i>Fluid Phase Equilibria</i> , 2019, 496, 17-30.	1.4	4
10	On the behavior of the osmotic second virial coefficients of gases in aqueous solutions: Rigorous results, accurate approximations, and experimental evidence. <i>Journal of Chemical Physics</i> , 2019, 150, 124503.	1.2	8
11	On the Solute-Induced Structure-Making/Breaking Effect: Rigorous Links among Microscopic Behavior, Solvation Properties, and Solution Non-Ideality. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2930-2947.	1.2	17
12	On fundamentally-based and thermodynamically-consistent description of dilute multicomponent solutions: Formal results, microscopic interpretations, and modeling implications. <i>Fluid Phase Equilibria</i> , 2018, 470, 2-16.	1.4	8
13	On the solubility of gases in dilute solutions: Organic food for thoughts from a molecular thermodynamic perspective. <i>Fluid Phase Equilibria</i> , 2018, 472, 94-106.	1.4	8
14	Gas solubility in dilute solutions: A novel molecular thermodynamic perspective. <i>Journal of Chemical Physics</i> , 2018, 148, 174502.	1.2	14
15	Toward the understanding of hydration phenomena in aqueous electrolytes from the interplay of theory, molecular simulation, and experiment. <i>Fluid Phase Equilibria</i> , 2016, 407, 84-104.	1.4	17
16	Can We Describe Graphene Confined Water Structures as Overlapping of Approaching Graphene's "Water Interfacial Structures?. <i>Journal of Physical Chemistry C</i> , 2016, 120, 7553-7561.	1.5	9
17	"Thought experiments" as dry-runs for "tough experiments": novel approaches to the hydration behavior of oxyanions. <i>Pure and Applied Chemistry</i> , 2016, 88, 163-176.	0.9	6
18	Single-ion hydration thermodynamics from clusters to bulk solutions: Recent insights from molecular modeling. <i>Fluid Phase Equilibria</i> , 2016, 407, 58-75.	1.4	32

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19	Rigorous force field optimization principles based on statistical distance minimization. Journal of Chemical Physics, 2015, 143, 144110.	1.2	14
20	NO <sub>3</sub> <sup>-</sup> Coordination in Aqueous Solutions by <sup>15</sup> N/ <sup>14</sup> N and <sup>18</sup> O/ <sup>16</sup> O Isotopic Substitution: What Can We Learn from Molecular Simulation?. Journal of Physical Chemistry B, 2015, 119, 519-531.	1.2	20
21	Thermodynamics of Small Alkali Metal Halide Cluster Ions: Comparison of Classical Molecular Simulations with Experiment and Quantum Chemistry. Journal of Physical Chemistry A, 2015, 119, 488-500.	1.1	7
22	Translational diffusion of water inside hydrophobic carbon micropores studied by neutron spectroscopy and molecular dynamics simulation. Physical Review E, 2015, 91, 022124.	0.8	16
23	Compounding effects of fluid confinement and surface strain on the wet-dry transition, thermodynamic response, and dynamics of water-graphene systems. Molecular Physics, 2015, 113, 1033-1042.	0.8	1
24	Vapor-Liquid Equilibrium and Polarization Behavior of the GCP Water Model: Gaussian Charge-on-Spring versus Dipole Self-Consistent Field Approaches to Induced Polarization. Journal of Physical Chemistry B, 2015, 119, 5010-5019.	1.2	18
25	Ewald Summation Approach to Potential Models of Aqueous Electrolytes Involving Gaussian Charges and Induced Dipoles: Formal and Simulation Results. Journal of Physical Chemistry B, 2014, 118, 13658-13670.	1.2	7
26	Surface Strain Effects on the Water-Graphene Interfacial and Confinement Behavior. Journal of Physical Chemistry C, 2014, 118, 19701-19711.	1.5	21
27	Sorption Phase of Supercritical CO <sub>2</sub> in Silica Aerogel: Experiments and Mesoscale Computer Simulations. Journal of Physical Chemistry C, 2014, 118, 15525-15533.	1.5	24
28	Correspondence between Cluster-Ion and Bulk Solution Thermodynamic Properties: On the Validity of the Cluster-Pair-Based Approximation. Journal of Physical Chemistry A, 2013, 117, 11328-11338.	1.1	39
29	Surface Corrugation Effects on the Water-Graphene Interfacial and Confinement Behavior. Journal of Physical Chemistry C, 2013, 117, 23875-23886.	1.5	20
30	Acid Gases in CO <sub>2</sub> -rich Subsurface Geologic Environments. Reviews in Mineralogy and Geochemistry, 2013, 77, 361-398.	2.2	14
31	10. Acid Gases in CO <sub>2</sub> -rich Subsurface Geologic Environments. , 2013, , 361-398.		2
32	Understanding controls on interfacial wetting at epitaxial graphene: Experiment and theory. Physical Review B, 2012, 85, .	1.1	95
33	Aqueous CO <sub>2</sub> Solutions at Silica Surfaces and within Nanopore Environments. Insights from Isobaric-Isothermal Molecular Dynamics. Journal of Physical Chemistry C, 2012, 116, 13904-13916.	1.5	26
34	Aqua Ions-Graphene Interfacial and Confinement Behavior: Insights from Isobaric-Isothermal Molecular Dynamics. Journal of Physical Chemistry A, 2011, 115, 5918-5927.	1.1	43
35	Optimized Unlike-Pair Interactions for Water-Carbon Dioxide Mixtures Described by the SPC/E and EPM2 Models. Journal of Physical Chemistry B, 2011, 115, 8775-8784.	1.2	68
36	On the molecular mechanism of surface charge amplification and related phenomena at aqueous polyelectrolyte-graphene interfaces. Condensed Matter Physics, 2011, 14, 33002.	0.3	10

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37	Modeling the effect of water vapor on the interfacial behavior of high-temperature air in contact with Fe <sub>20</sub> Cr surfaces. <i>Scripta Materialia</i> , 2011, 64, 1027-1030.	2.6	6
38	Solvation and ion pair association in aqueous metal sulfates: Interpretation of NDIS raw data by isobaric isothermal molecular dynamics simulation. <i>Collection of Czechoslovak Chemical Communications</i> , 2010, 75, 405-424.	1.0	10
39	Polarization behavior of water in extreme aqueous environments: A molecular dynamics study based on the Gaussian charge polarizable water model. <i>Journal of Chemical Physics</i> , 2010, 133, 074504.	1.2	19
40	Supercritical fluid behavior at nanoscale interfaces: Implications for CO <sub>2</sub> sequestration in geologic formations. <i>Philosophical Magazine</i> , 2010, 90, 2339-2363.	0.7	111
41	Ion-Pair Association in Ultrasupercritical Aqueous Environments: Successful Interplay among Conductance Experiments, Theory, and Molecular Simulations. <i>Journal of Chemical &amp; Engineering Data</i> , 2010, 55, 1828-1836.	1.0	16
42	Ion Pair Association in Extreme Aqueous Environments: Molecular-based and Electrical Conductance Approaches. <i>Journal of Solution Chemistry</i> , 2009, 38, 827-841.	0.6	14
43	Liquid-vapor equilibrium isotopic fractionation of water: How well can classical water models predict it?. <i>Journal of Chemical Physics</i> , 2009, 130, 094509.	1.2	16
44	On the Molecular-Based Modeling of Dilute Ternary Systems in Compressible Media: Formal Results and Thermodynamic Pitfalls. <i>ACS Symposium Series</i> , 2009, , 66-80.	0.5	1
45	Molecular Dynamics Simulation of the Interfacial Behavior of Short-Chain Polystyrene Sulfonate Aqueous Solutions in Contact with Graphene Surfaces in the Presence of Multivalent Cations. <i>Journal of Physical Chemistry C</i> , 2008, 112, 19521-19529.	1.5	33
46	Solvation phenomena in dilute multicomponent solutions I. Formal results and molecular outlook. <i>Journal of Chemical Physics</i> , 2008, 128, 214512.	1.2	9
47	Molecular-Based Modeling of Water and Aqueous Solutions at Supercritical Conditions. <i>Advances in Chemical Physics</i> , 2007, , 115-205.	0.3	61
48	Novel Corresponding-States Principle Approach for the Equation of State of Isotopologues: H <sub>2</sub> O as an Example. <i>Journal of Physical Chemistry B</i> , 2007, 111, 393-401.	1.2	11
49	H <sub>3</sub> O <sup>+</sup> Cl <sup>-</sup> Pair Association in Steam and Highly Compressible Aqueous Environments. <i>Journal of Physical Chemistry C</i> , 2007, 111, 15569-15574.	1.5	12
50	Testing the adequacy of simple water models at the opposite ends of the phase diagram. <i>Journal of Molecular Liquids</i> , 2007, 134, 94-98.	2.3	7
51	Ion pairing and counterion condensation in aqueous electrolyte and polyelectrolyte solutions: Insights from molecular simulation. <i>Journal of Molecular Liquids</i> , 2007, 134, 15-22.	2.3	15
52	Simulated water adsorption in chemically heterogeneous carbon nanotubes. <i>Journal of Chemical Physics</i> , 2006, 124, 074710.	1.2	76
53	On the re-engineered TIP4P water models for the prediction of vapor-liquid equilibrium. <i>Journal of Molecular Liquids</i> , 2006, 129, 120-124.	2.3	19
54	Limitations of the rigid planar nonpolarizable models of water. <i>Journal of Chemical Physics</i> , 2006, 124, 074507.	1.2	24

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55	Liquid-vapor isotopic fractionation factors of diatomic fluids: A direct comparison between molecular simulation and experiment. <i>Journal of Chemical Physics</i> , 2006, 125, 034510.	1.2	5
56	Ion association in aqueous LiCl solutions at high concentration: Predicted results via molecular simulation. <i>Journal of Chemical Physics</i> , 2006, 124, 154509.	1.2	23
57	The Effect of Pore Connectivity on Water Adsorption Isotherms in Non-Activated Graphitic Nanopores. <i>Adsorption</i> , 2005, 11, 337-341.	1.4	17
58	Simulated Water Adsorption Isotherms in Hydrophilic and Hydrophobic Cylindrical Nanopores. <i>Adsorption</i> , 2005, 11, 397-401.	1.4	43
59	From dimer to condensed phases at extreme conditions: Accurate predictions of the properties of water by a Gaussian charge polarizable model. <i>Journal of Chemical Physics</i> , 2005, 122, 244511.	1.2	202
60	Vapor-liquid equilibria and thermophysical behavior of the SPC-HW model for heavy water. <i>Molecular Simulation</i> , 2005, 31, 1035-1042.	0.9	0
61	Computer simulation of the 13 crystalline phases of ice. <i>Journal of Chemical Physics</i> , 2005, 123, 054502.	1.2	29
62	Solvation Behavior of Short-Chain Polystyrene Sulfonate in Aqueous Electrolyte Solutions: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 23031-23042.	1.2	40
63	Effect of the Range of Interactions on the Properties of Fluids. 2. Structure and Phase Behavior of Acetonitrile, Hydrogen Fluoride, and Formic Acid. <i>Journal of Physical Chemistry B</i> , 2005, 109, 9736-9750.	1.2	17
64	Effect of Temperature on the Adsorption of Water in Porous Carbons. <i>Langmuir</i> , 2005, 21, 9457-9467.	1.6	87
65	Water in carbon nanotubes: Adsorption isotherms and thermodynamic properties from molecular simulation. <i>Journal of Chemical Physics</i> , 2005, 122, 234712.	1.2	225
66	The effect of salt concentration on the structure of water in CaCl <sub>2</sub> aqueous solutions. <i>Journal of Molecular Liquids</i> , 2004, 112, 99-99.	2.3	1
67	Simulated water adsorption isotherms in carbon nanopores. <i>Molecular Physics</i> , 2004, 102, 243-251.	0.8	91
68	Electric Double Layer at the Rutile (110) Surface. 1. Structure of Surfaces and Interfacial Water from Molecular Dynamics by Use of ab Initio Potentials. <i>Journal of Physical Chemistry B</i> , 2004, 108, 12049-12060.	1.2	272
69	Ion Adsorption at the Rutile-Water Interface: Linking Molecular and Macroscopic Properties. <i>Langmuir</i> , 2004, 20, 4954-4969.	1.6	298
70	H <sub>3</sub> O <sup>+</sup> /Cl <sup>-</sup> ion pairing in hydrothermal solutions by simulation and electrical conductance. A review. <i>Journal of Molecular Liquids</i> , 2003, 103-104, 235-248.	2.3	10
71	The structure of CaCl <sub>2</sub> aqueous solutions over a wide range of concentration. Interpretation of diffraction experiments via molecular simulation. <i>Journal of Chemical Physics</i> , 2003, 119, 8052-8061.	1.2	97
72	Water Adsorption in Carbon-Slit Nanopores. <i>Langmuir</i> , 2003, 19, 8583-8591.	1.6	212

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73	Isotopic effect on phase equilibria of atomic fluids and their mixtures: A direct comparison between molecular simulation and experiment. <i>Journal of Chemical Physics</i> , 2003, 119, 4458-4467.	1.2	17
74	Aqueous Na+Cl <sup>-</sup> pair association from liquidlike to steamlike densities along near-critical isotherms. <i>Journal of Chemical Physics</i> , 2003, 118, 7921-7929.	1.2	43
75	Microstructure of Water At the Level of Three-particle Correlation Functions As Predicted by Classical Intermolecular Models. <i>Molecular Simulation</i> , 2003, 29, 13-21.	0.9	10
76	Pair approximation for polarization interaction and adiabatic nuclear and electronic sampling method for fluids with dipole polarizability. <i>Molecular Physics</i> , 2002, 100, 2703-2717.	0.8	14
77	Determination of the Gibbs Free Energy of Gas Replacement in SI Clathrate Hydrates by Molecular Simulation. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7982-7987.	1.1	101
78	H <sub>3</sub> O <sup>+</sup> /Cl <sup>-</sup> Association in High-Temperature Aqueous Solutions over a Wide Range of State Conditions. A Direct Comparison between Simulation and Electrical Conductance Experiment. <i>Journal of Physical Chemistry B</i> , 2002, 106, 2041-2046.	1.2	28
79	The structure of concentrated NiCl <sub>2</sub> aqueous solutions: what is molecular simulation revealing about the neutron scattering methodologies?. <i>Molecular Physics</i> , 2002, 100, 2307-2315.	0.8	21
80	Molecular Dynamics Study of the Structure and Thermophysical Properties of Model si Clathrate Hydrates. <i>Journal of Physical Chemistry B</i> , 2002, 106, 442-451.	1.2	109
81	Effect of the Range of Interactions on the Properties of Fluids. Phase Equilibria in Pure Carbon Dioxide, Acetone, Methanol, and Water. <i>Journal of Physical Chemistry B</i> , 2002, 106, 7537-7546.	1.2	48
82	Vapor-liquid equilibrium simulations of the SCPDP model of water. <i>Chemical Physics Letters</i> , 2002, 357, 189-194.	1.2	56
83	Solvation in high-temperature electrolyte solutions. III. Integral equation calculations and interpretation of experimental data. <i>Journal of Chemical Physics</i> , 2001, 114, 3575-3585.	1.2	19
84	Pair approximation for polarization interaction: efficient method for Monte Carlo simulations of polarizable fluids. <i>Molecular Physics</i> , 2001, 99, 349-354.	0.8	20
85	Examination of Chain Length Effects on the Solubility of Alkanes in Near-Critical and Supercritical Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , 2001, 105, 841-847.	1.2	31
86	Chain length effects on aqueous alkane solubility near the solvent's critical point. <i>Fluid Phase Equilibria</i> , 2001, 183-184, 289-294.	1.4	3
87	On the determination of the vapor-liquid envelope for polarizable models by Monte Carlo simulation. <i>Fluid Phase Equilibria</i> , 2001, 183-184, 295-300.	1.4	7
88	On the determination of orientational configurational temperature from computer simulation. <i>Journal of Chemical Physics</i> , 2001, 114, 6514-6517.	1.2	12
89	Solvation in high-temperature aqueous electrolyte solutions. <i>Journal of Molecular Liquids</i> , 2000, 87, 233-242.	2.3	2
90	The structure of water from 25°C to 457°C: comparison between neutron scattering and molecular simulation. <i>Chemical Physics</i> , 2000, 258, 109-120.	0.9	40

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91	Applications of Integral Equation Calculations to High-Temperature Solvation Phenomena. Journal of Statistical Physics, 2000, 100, 167-199.	0.5	12
92	Molecular Simulation and Modeling of Supercritical Water and Aqueous Solutions. , 2000, , 345-394.		1
93	Molecular approach to high-temperature solvation. Formal, integral equation and experimental results. Journal of Physics Condensed Matter, 2000, 12, 3585-3593.	0.7	17
94	H <sub>3</sub> O <sup>+</sup> /Cl <sup>-</sup> ion-pair formation in high-temperature aqueous solutions. Journal of Chemical Physics, 2000, 113, 8093-8100.	1.2	36
95	Solvation in high-temperature electrolyte solutions. II. Some formal results. Journal of Chemical Physics, 1999, 110, 1075-1086.	1.2	51
96	Solvation in high-temperature electrolyte solutions. I. Hydration shell behavior from molecular simulation. Journal of Chemical Physics, 1999, 110, 1064-1074.	1.2	45
97	Solvation effect on kinetic rate constant of reactions in supercritical solvents. AIChE Journal, 1998, 44, 667-680.	1.8	42
98	Simple transferable intermolecular potential for the molecular simulation of water over wide ranges of state conditions. Fluid Phase Equilibria, 1998, 150-151, 73-81.	1.4	64
99	Thermodynamics and kinetics of ion speciation in supercritical aqueous solutions: a molecular-based study. Fluid Phase Equilibria, 1998, 150-151, 107-115.	1.4	16
100	Interplay between Molecular Simulation and Neutron Scattering in Developing New Insights into the Structure of Water. Industrial & Engineering Chemistry Research, 1998, 37, 3021-3025.	1.8	37
101	Molecular simulation study of speciation in supercritical aqueous NaCl solutions. Journal of Molecular Liquids, 1997, 73-74, 361-372.	2.3	32
102	Temperature and density effects on the high temperature ionic speciation in dilute Na <sup>+</sup> /Cl <sup>-</sup> aqueous solutions. Journal of Chemical Physics, 1996, 105, 9248-9257.	1.2	48
103	Solvation structure, hydrogen bonding, and ion pairing in dilute supercritical aqueous NaCl mixtures. International Journal of Thermophysics, 1996, 17, 147-156.	1.0	10
104	Solvation thermodynamics of gas solubility at sub- and near-critical conditions. AIChE Journal, 1996, 42, 571-584.	1.8	34
105	Engineering a simple polarizable model for the molecular simulation of water applicable over wide ranges of state conditions. Journal of Chemical Physics, 1996, 105, 8274-8281.	1.2	151
106	On the realism of the re-engineered simple point charge water model. Journal of Chemical Physics, 1996, 104, 5240-5243.	1.2	14
107	Microstructure of Ambient and Supercritical Water. Direct Comparison between Simulation and Neutron Scattering Experiments. The Journal of Physical Chemistry, 1996, 100, 1309-1316.	2.9	129
108	Molecular simulation of supercritical water and aqueous solutions. Journal of Physics Condensed Matter, 1996, 8, 9281-9287.	0.7	12



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109	Molecular-Based Approach to Gas Solubility at Near-Critical Conditions. ACS Symposium Series, 1995, , 34-46.	0.5	3
110	Na+â€œClâ€™ion pair association in supercritical water. Journal of Chemical Physics, 1995, 103, 9379-9387.	1.2	141
111	Comment on â€œNear critical phase behaviour of dilute mixturesâ€™. Molecular Physics, 1995, 84, 41-48.	0.8	52
112	Hydrogen bonding in supercritical water. Journal of Chemical Physics, 1994, 101, 4466-4469.	1.2	121
113	Molecular simulation study of solvation structure in supercritical aqueous solutions. Chemical Engineering Science, 1994, 49, 2735-2748.	1.9	79
114	Solute-induced effects on the structure and thermodynamics of infinitely dilute mixtures. AIChE Journal, 1994, 40, 1558-1573.	1.8	172
115	Accurate calculation of excess thermal, infinite dilution, and related properties of liquid mixtures via molecular-based simulation. Fluid Phase Equilibria, 1993, 83, 23-32.	1.4	31
116	Structure of Mixed Solvent Electrolyte Solutions via Gibbs Ensemble Monte Carlo Simulation. Molecular Simulation, 1993, 11, 163-175.	0.9	6
117	Relationship between McQuarrie and Helfand equations for the determination of shear viscosity from equilibrium molecular dynamics. Physical Review E, 1993, 47, 1702-1711.	0.8	8
118	Solute-solute and solute-solvent correlations in dilute near-critical ternary mixtures: mixed-solute and entrainer effects. The Journal of Physical Chemistry, 1993, 97, 2740-2744.	2.9	68
119	Unified expression for the calculation of thermal conductivity in the canonical ensemble. Molecular Physics, 1993, 78, 791-797.	0.8	0
120	Soluteâ€œsolute correlations in infinitely dilute supercritical mixtures. Journal of Chemical Physics, 1992, 97, 504-507.	1.2	29
121	Local Density Augmentation in Supercritical Solutions. ACS Symposium Series, 1992, , 60-72.	0.5	43
122	Molecular dynamics study of solute-solute microstructure in attractive and repulsive supercritical mixtures. Industrial & Engineering Chemistry Research, 1992, 31, 1391-1397.	1.8	54
123	An automated Verlet neighbor list algorithm with a multiple time-step approach for the simulation of large systems. Computer Physics Communications, 1992, 70, 467-477.	3.0	9
124	A Study of Solute-Solvent Interactions at Infinite Dilution via the Coupling Parameter Approach. Molecular Simulation, 1991, 7, 265-283.	0.9	8
125	On the performance of an automated Verlet neighbor list algorithm for large systems on a vector processor. Computer Physics Communications, 1991, 64, 15-18.	3.0	18
126	Determination of excess Gibbs free energy by the single-charging-integral approach. Infinite dilution activity coefficients and related quantities. The Journal of Physical Chemistry, 1991, 95, 6683-6687.	2.9	24



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127	Use of the McQuarrie equation for the computation of shear viscosity via equilibrium molecular dynamics. <i>Physical Review A</i> , 1991, 43, 4289-4295.	1.0	23
128	Excess properties of liquid mixtures from computer simulation: a coupling-parameter approach to the determination of their dependence on molecular asymmetry. <i>Molecular Physics</i> , 1991, 73, 127-140.	0.8	24
129	On the use of the Verlet neighbor list in molecular dynamics. <i>Computer Physics Communications</i> , 1990, 60, 215-224.	3.0	46
130	Determination of excess Gibbs free energy from computer simulation by the single charging integral approach. I. Theory. <i>Journal of Chemical Physics</i> , 1990, 92, 673-679.	1.2	50
131	A molecular dynamics study of the influence of elongation and quadrupole moment upon some thermodynamic and transport properties of linear heteronuclear triatomic fluids. <i>Journal of Chemical Physics</i> , 1989, 91, 7818-7830.	1.2	6
132	The influence of unlike molecule interaction parameters on liquid mixture excess properties. <i>Fluid Phase Equilibria</i> , 1989, 48, 161-176.	1.4	20
133	Thermodynamic excess properties in binary fluid mixtures. <i>Industrial &amp; Engineering Chemistry Research</i> , 1988, 27, 664-671.	1.8	16
134	Determination of Excess Gibbs Free Energy from Computer Simulation: Multiple-Parameter Charging Approach. <i>Fluid Phase Equilibria</i> , 1987, 37, 293-303.	1.4	21
135	DISCREPANCY IN THE DETERMINATION OF THE ACTIVATION ENERGY BY CATALYTIC WIRE TECHNIQUES, NH <sub>3</sub> OXIDATION. <i>Chemical Engineering Communications</i> , 1986, 41, 271-277.	1.5	0
136	Molecular-Based Description of the Osmotic Second Virial Coefficients of Electrolytes: Rigorous Formal Links to Solute-Solvent Interaction Asymmetry, Virial Expansion Paths, and Experimental Evidence. <i>Journal of Physical Chemistry B</i> , 0, , .	1.2	4