David A Kofke

List of Publications by Year
in descending order

172 papers	6,932 citations	70961 41 h-index	66788 78 g-index
180 all docs	180 docs citations	180 times ranked	3166 citing authors

#	Article	IF	Citations
1	The Journal of Chemical & Engineering Data: Introduction of Topical Sections and Updates from the Editorial Team. Journal of Chemical & Engineering Data, 2022, 67, 1-2.	1.0	1
2	Identifying and estimating bias in overlap-sampling free-energy calculations. Molecular Simulation, 2021, 47, 379-389.	0.9	4
3	pyHMA: A VASP post-processor for precise measurement of crystalline anharmonic properties using harmonically mapped averaging. Computer Physics Communications, 2021, 258, 107554.	3.0	4
4	Properties of supercritical N 2 , O 2 , CO 2 , and NH 3 mixtures from the virial equation of state. AICHE Journal, 2021, 67, e17072.	1.8	3
5	Journal of Chemical & Engineering Data: An Update from the Editorial Team. Journal of Chemical & Engineering Data, 2021, 66, 1-2.	1.0	0
6	Journal of Chemical & Engineering Data: Why Change the Cover Page?. Journal of Chemical & Engineering Data, 2021, 66, 859-860.	1.0	0
7	Historical Perspective of the Journal of Chemical & Engineering Dataâ€™s Published Topics, 1956â€“2020. Journal of Chemical & Engineering Data, 2021, 66, 1555-1556.	1.0	1
8	Evaluation of Osmotic Virial Coefficients via Restricted Gibbs Ensemble Simulations, with Support from Gas-Phase Mixture Coefficients. Journal of Physical Chemistry B, 2021, 125, 7262-7272.	1.2	1
9	Speed of Sound in Helium-4 from Ab Initio Acoustic Virial Coefficients. Journal of Chemical & Engineering Data, 2021, 66, 3258-3281.	1.0	8
10	Molecular Calculation of the Critical Parameters of Classical Helium. Journal of Chemical & Engineering Data, 2020, 65, 1028-1037.	1.0	6
11	Implementation of harmonically mapped averaging in LAMMPS, and effect of potential truncation on anharmonic properties. Journal of Chemical Physics, 2020, 152, 014107.	1.2	3
12	Cluster integrals and virial coefficients for realistic molecular models. Physical Review E, 2020, 101, 051301.	0.8	9
13	Highlighting 10 Years of NIST Cooperation and Service to the Thermophysical Properties Data Community. Journal of Chemical & Engineering Data, 2019, 64, 4191-4192.	1.0	4
14	Alternative ensemble averages in molecular dynamics simulation of hard spheres. Molecular Physics, 2019, 117, 3734-3753.	0.8	4
15	Force-sampling methods for density distributions as instances of mapped averaging. Molecular Physics, 2019, 117, 2822-2829.	0.8	15
16	Virial Coefficients of Helium-4 from Ab Initio-Based Molecular Models. Journal of Chemical & Engineering Data, 2019, 64, 3742-3754.	1.0	17
17	Introducing JCEDâ€™s Latin America Special Issue. Journal of Chemical & Engineering Data, 2019, 64, 1859-1859.	1.0	1
18	Alternatives to conventional ensemble averages for thermodynamic properties. Current Opinion in Chemical Engineering, 2019, 23, 70-76.	3.8	11

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19	Combined temperature and density series for fluid-phase properties. II. Lennard-Jones spheres. Journal of Chemical Physics, 2019, 151, 204501.	1.2	13
20	Molecular Calculation of the Critical Parameters of Classical Helium. Journal of Chemical & Engineering Data, 2019, 65, .	1.0	0
21	Electric-field mapped averaging for the dielectric constant. Fluid Phase Equilibria, 2018, 470, 17-24.	1.4	2
22	Comprehensive high-precision high-accuracy equation of state and coexistence properties for classical Lennard-Jones crystals and low-temperature fluid phases. Journal of Chemical Physics, 2018, 149, 204508.	1.2	43
23	Effects of thermostatting in molecular dynamics on anharmonic properties of crystals: Application to fcc Al at high pressure and temperature. Journal of Chemical Physics, 2018, 149, 124109.	1.2	16
24	Peer Review Appreciation at JCED. Journal of Chemical & Engineering Data, 2018, 63, 3169-3169.	1.0	1
25	Free energy and concentration of crystalline vacancies by molecular simulation. Molecular Physics, 2018, 116, 3027-3041.	0.8	9
26	No system-size anomalies in entropy of bcc iron at Earthâ€™s inner-core conditions. Scientific Reports, 2018, 8, 7295.	1.6	7
27	Quantum virial coefficients of molecular nitrogen. Molecular Physics, 2017, 115, 869-878.	0.8	6
28	Direct orientation sampling of diatomic molecules for path integral Monte Carlo calculation of fully quantum virial coefficients. Journal of Chemical Physics, 2017, 146, .	1.2	4
29	Evaluation of second and third dielectric virial coefficients for non-polarisable molecular models. Molecular Physics, 2017, 115, 991-1003.	0.8	7
30	Harmonically Assisted Methods for Computing the Free Energy of Classical Crystals by Molecular Simulation: A Comparative Study. Journal of Chemical Theory and Computation, 2017, 13, 825-834.	2.3	20
31	Virial Coefficients and Equations of State for Hard Polyhedron Fluids. Langmuir, 2017, 33, 11788-11796.	1.6	19
32	Accurate and precise ab initio anharmonic free-energy calculations for metallic crystals: Application to hcp Fe at high temperature and pressure. Physical Review B, 2017, 96, .	1.1	25
33	Quantum Virial Coefficients via Path Integral Monte Carlo with Semi-classical Beads. Molecular Modeling and Simulation, 2016, , 93-106.	0.2	0
34	Reformulation of Ensemble Averages via Coordinate Mapping. Journal of Chemical Theory and Computation, 2016, 12, 1491-1498.	2.3	24
35	Calculation of high-order virial coefficients for the square-well potential. Physical Review E, 2016, 94, 013301.	0.8	8
36	Thermodynamic Properties of Supercritical CO₂/CH₄ Mixtures from the Virial Equation of State. Journal of Chemical & Engineering Data, 2016, 61, 4296-4312.	1.0	9

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37	Vapor-phase metastability and condensation via the virial equation of state with extrapolated coefficients. Fluid Phase Equilibria, 2016, 409, 12-18.	1.4	20
38	Very fast averaging of thermal properties of crystals by molecular simulation. Physical Review E, 2015, 92, 043303.	0.8	27
39	Eighth to sixteenth virial coefficients of the Lennard-Jones model. Journal of Chemical Physics, 2015, 143, 044504.	1.2	33
40	Communication: Analytic continuation of the virial series through the critical point using parametric approximants. Journal of Chemical Physics, 2015, 143, 071103.	1.2	21
41	Molecularâ€based virial coefficients of CO₂â€H₂O mixtures. AICHE Journal, 2015, 61, 3029-3037.	1.8	15
42	Etomica: An objectâ€oriented framework for molecular simulation. Journal of Computational Chemistry, 2015, 36, 573-583.	1.5	22
43	The rate of convergence of the virial series in confined systems. Molecular Physics, 2015, 113, 1179-1189.	0.8	8
44	Combined temperature and density series for fluid-phase properties. I. Square-well spheres. Journal of Chemical Physics, 2015, 143, 114110.	1.2	12
45	Effects of Finite Size and Proton Disorder on Lattice-Dynamics Estimates of the Free Energy of Clathrate Hydrates. Industrial & Engineering Chemistry Research, 2015, 54, 4487-4496.	1.8	6
46	Mixed-precision models for calculation of high-order virial coefficients on GPUs. , 2014, , .		0
47	Fifth to eleventh virial coefficients of hard spheres. Physical Review E, 2014, 90, 023301.	0.8	59
48	Quantifying Computational Effort Required for Stochastic Averages. Journal of Chemical Theory and Computation, 2014, 10, 5229-5234.	2.3	23
49	Critical isotherms from virial series using asymptotically consistent approximants. AICHE Journal, 2014, 60, 3336-3349.	1.8	19
50	Interpreting Gas-Saturation Vapor-Pressure Measurements Using Virial Coefficients Derived from Molecular Models. Journal of Chemical & Engineering Data, 2014, 59, 3183-3192.	1.0	7
51	A comparative study of methods to compute the free energy of an ordered assembly by molecular simulation. Journal of Chemical Physics, 2013, 139, 084105.	1.2	18
52	Mayer Sampling Monte Carlo calculation of virial coefficients on graphics processors. Molecular Physics, 2013, 111, 535-543.	0.8	28
53	Second through fifth virial coefficients for model methaneâ€“ethane mixtures. Fluid Phase Equilibria, 2013, 351, 69-73.	1.4	10
54	Calculation of inhomogeneous-fluid cluster expansions with application to the hard-sphere/hard-wall system. Journal of Chemical Physics, 2013, 138, 134706.	1.2	19

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55	Path-integral Mayer-sampling calculations of the quantum Boltzmann contribution to virial coefficients of helium-4. Journal of Chemical Physics, 2012, 137, 184101.	1.2	42
56	Solder joint grain boundary structure and diffusivity via molecular dynamics simulations. , 2012, , .		0
57	Virial Equation of State of Water Based on Wertheimâ€™s Association Theory. Journal of Physical Chemistry B, 2012, 116, 14078-14088.	1.2	9
58	Semiclassical fifth virial coefficients for improved ab initio helium-4 standards. Chemical Physics Letters, 2012, 531, 11-17.	1.2	28
59	Solute Effects on Î²-Sn Grain Boundary Energy and Shear Stress. Journal of Nanomechanics & Micromechanics, 2011, 1, 41-50.	1.4	9
60	Virial coefficients, equation of state, and solidâ€“fluid coexistence for the soft sphere model. Molecular Physics, 2011, 109, 123-132.	0.8	21
61	Efficient calculation of Î±- and Î²-nitrogen free energies and coexistence conditions via overlap sampling with targeted perturbation. Journal of Chemical Physics, 2011, 135, 044125.	1.2	9
62	Integral-equation theories and Mayer-sampling Monte Carlo: a tandem approach for computing virial coefficients of simple fluids. Molecular Physics, 2011, 109, 2395-2406.	0.8	15
63	Mayer-sampling Monte Carlo calculations of uniquely flexible contributions to virial coefficients. Journal of Chemical Physics, 2011, 135, 124101.	1.2	27
64	Algorithm for constant-pressure Monte Carlo simulation of crystalline solids. Physical Review E, 2011, 84, 046712.	0.8	6
65	Effect of Cu and Ag solute segregation on Î²Sn grain boundary diffusivity. Journal of Applied Physics, 2011, 110, 013528.	1.1	18
66	Modeling solubility in supercritical fluids via the virial equation of state. Journal of Supercritical Fluids, 2010, 55, 479-484.	1.6	10
67	Atomistic modeling of Î²-Sn surface energies and adatom diffusivity. Applied Surface Science, 2010, 256, 4402-4407.	3.1	44
68	Mayer-sampling Monte Carlo calculations of methanol virial coefficients. Molecular Simulation, 2010, 36, 1282-1288.	0.9	7
69	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î²</mml:mi><mml:mtext>-Sn</mml:mtext></mml:mrow></mml:math>grain-boundary structure and self-diffusivity via molecular dynamics simulations. Physical Review B, 2010, 81, .	1.1	35
70	Suitability of umbrella- and overlap-sampling methods for calculation of solid-phase free energies by molecular simulation. Journal of Chemical Physics, 2010, 132, 214103.	1.2	19
71	Efficient calculation of temperature dependence of solid-phase free energies by overlap sampling coupled with harmonically targeted perturbation. Journal of Chemical Physics, 2010, 133, 134104.	1.2	21
72	Molecular Based Modeling of Associating Fluids via Calculation of Wertheim Cluster Integrals. Journal of Physical Chemistry B, 2010, 114, 11515-11524.	1.2	5

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73	Virial coefficients of model alkanes. Journal of Chemical Physics, 2010, 133, 104101.	1.2	40
74	The effect of truncation and shift on virial coefficients of Lennardâ€“Jones potentials. Collection of Czechoslovak Chemical Communications, 2010, 75, 447-462.	1.0	21
75	Lattice Strain Due to an Atomic Vacancy. International Journal of Molecular Sciences, 2009, 10, 2798-2808.	1.8	40
76	Virial coefficients of Lennard-Jones mixtures. Journal of Chemical Physics, 2009, 130, 224104.	1.2	14
77	Fourth and Fifth Virial Coefficients of Polarizable Water. Journal of Physical Chemistry B, 2009, 113, 7810-7815.	1.2	51
78	Sixth, seventh and eighth virial coefficients of the Lennard-Jones model. Molecular Physics, 2009, 107, 2309-2318.	0.8	66
79	Interpolation of virial coefficients. Molecular Physics, 2009, 107, 1431-1436.	0.8	10
80	Semigrand Canonical Monte Carlo Simulation; Integration Along Coexistence Lines. Advances in Chemical Physics, 2007, , 405-441.	0.3	39
81	Calculation of surface tension via area sampling. Journal of Chemical Physics, 2007, 127, 174709.	1.2	99
82	Virial Coefficients of Polarizable Water:â€‰ Applications to Thermodynamic Properties and Molecular Clustering. Journal of Physical Chemistry C, 2007, 111, 16021-16027.	1.5	50
83	Higher-Order Virial Coefficients of Water Models. Journal of Physical Chemistry B, 2007, 111, 11463-11473.	1.2	78
84	Gas-Phase Molecular Clustering of TIP4P and SPC/E Water Models from Higher-Order Virial Coefficients. Industrial & Engineering Chemistry Research, 2006, 45, 5566-5573.	1.8	43
85	On the sampling requirements for exponential-work free-energy calculations. Molecular Physics, 2006, 104, 3701-3708.	0.8	32
86	Three-body effects in hydrogen fluoride: survey of potential energy surfaces. Molecular Physics, 2006, 104, 503-513.	0.8	7
87	Free energy methods in molecular simulation. Fluid Phase Equilibria, 2005, 228-229, 41-48.	1.4	87
88	Phase-space overlap measures. II. Design and implementation of staging methods for free-energy calculations. Journal of Chemical Physics, 2005, 123, 084109.	1.2	95
89	Evaluation of bridge-function diagrams via Mayer-sampling Monte Carlo simulation. Journal of Chemical Physics, 2005, 122, 104508.	1.2	16
90	Effect of monovacancies on the relative stability of fcc and hcp hard-sphere crystals. Journal of Chemical Physics, 2005, 122, 176101.	1.2	6

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91	Rosenbluth-sampled nonequilibrium work method for calculation of free energies in molecular simulation. Journal of Chemical Physics, 2005, 122, 204104.	1.2	45
92	Trimer Based Polarization as a Multibody Molecular Model. Application to Hydrogen Fluoride. Journal of the American Chemical Society, 2005, 127, 690-698.	6.6	5
93	Molecular Simulation Study of the Effect of Pressure on the Vaporâ^'Liquid Interface of the Square-Well Fluid. Langmuir, 2005, 21, 4218-4226.	1.6	9
94	Phase-space overlap measures. I. Fail-safe bias detection in free energies calculated by molecular simulation. Journal of Chemical Physics, 2005, 123, 054103.	1.2	131
95	Selection of temperature intervals for parallel-tempering simulations. Journal of Chemical Physics, 2005, 122, 206101.	1.2	136
96	Perspective: Free Energies and Phase Equilibria. , 2005, , 683-705.		5
97	Perspective: Free Energies and Phase Equilibria. , 2005, , 683-705.		1
98	Model for small-sample bias of free-energy calculations applied to Gaussian-distributed nonequilibrium work measurements. Journal of Chemical Physics, 2004, 121, 8742-8747.	1.2	44
99	Getting the most from molecular simulation. Molecular Physics, 2004, 102, 405-420.	0.8	49
100	Molecular simulation study of miscibility in InxGa1â^'xN ternary alloys. Journal of Applied Physics, 2004, 95, 4500-4502.	1.1	30
101	Elastic constants and the effect of strain on monovacancy concentration in fcc hard-sphere crystals. Physical Review B, 2004, 70, .	1.1	8
102	Comment on â€œThe incomplete beta function law for parallel tempering sampling of classical canonical systemsâ€•[J. Chem. Phys. 120, 4119 (2004)]. Journal of Chemical Physics, 2004, 121, 1167-1167.	1.2	36
103	Improving the efficiency and reliability of free energy perturbation calculations using overlap sampling methods. Journal of Computational Chemistry, 2004, 25, 28-40.	1.5	145
104	Mayer Sampling: Calculation of Cluster Integrals using Free-Energy Perturbation Methods. Physical Review Letters, 2004, 92, 220601.	2.9	156
105	Asymmetric bias in free-energy perturbation measurements using two Hamiltonian-based models. Physical Review E, 2004, 70, 066702.	0.8	30
106	Using overlap and funnel sampling to obtain accurate free energies from nonequilibrium work measurements. Physical Review E, 2004, 69, 057702.	0.8	37
107	Liquid-Phase Activity Coefficients for Saturated HF/H2O Mixtures with Vapor-Phase Nonidealities Described by Molecular Simulation. Industrial & Engineering Chemistry Research, 2004, 43, 218-227.	1.8	4
108	Molecular simulation study of effect of molecular association on vapor-liquid interfacial properties. Journal of Chemical Physics, 2004, 121, 9574-9580.	1.2	30

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109	Molecular simulation study of miscibility of ternary and quaternary InGaAlN alloys. Journal of Applied Physics, 2004, 95, 6129-6137.	1.1	35
110	Molecular Simulation Study of the Vaporâ€“Liquid Interfacial Behavior of a Dimer-forming Associating Fluid. Molecular Simulation, 2004, 30, 343-351.	0.9	21
111	Staging Is More Important than Perturbation Method for Computation of Enthalpy and Entropy Changes in Complex Systems. Journal of Physical Chemistry B, 2003, 107, 5598-5611.	1.2	45
112	Surface tension and vaporâ€“liquid phase coexistence of the square-well fluid. Journal of Chemical Physics, 2003, 119, 3405-3412.	1.2	134
113	Fugacity Coefficients of Saturated Water from Molecular Simulation. Journal of Physical Chemistry B, 2003, 107, 12808-12813.	1.2	11
114	Hydrogen fluoride phase behavior and molecular structure: Ab initio derived potential models. Journal of Chemical Physics, 2003, 119, 6092-6099.	1.2	17
115	Appropriate methods to combine forward and reverse free-energy perturbation averages. Journal of Chemical Physics, 2003, 118, 2977-2984.	1.2	174
116	Variational formula for the free energy based on incomplete sampling in a molecular simulation. Physical Review E, 2003, 68, 026122.	0.8	14
117	Hydrogen fluoride phase behavior and molecular structure: A QM/MM potential model approach. Journal of Chemical Physics, 2003, 119, 7365-7371.	1.2	26
118	Self-referential method for calculation of the free energy of crystals by Monte Carlo simulation. Physical Review E, 2002, 65, 036709.	0.8	8
119	On the acceptance probability of replica-exchange Monte Carlo trials. Journal of Chemical Physics, 2002, 117, 6911-6914.	1.2	200
120	A comparison of some variational formulas for the free energy as applied to hard-sphere crystals. Journal of Chemical Physics, 2002, 117, 9111-9115.	1.2	3
121	Monte Carlo and cell model calculations for the solidâ€”fluid phase behaviour of the triangle-well model. Molecular Physics, 2002, 100, 1543-1550.	0.8	14
122	Improved models for the phase behaviour of hydrogen fluoride: chain and ring aggregates in the SAFT approach and the AEOS model. Molecular Physics, 2002, 100, 2241-2259.	0.8	49
123	UB association bias algorithm applied to the simulation of hydrogen fluoride. Fluid Phase Equilibria, 2002, 194-197, 249-256.	1.4	8
124	Free-energy calculations for fluid and solid phases by molecular simulation. Fluid Phase Equilibria, 2002, 194-197, 219-226.	1.4	3
125	Web-based technologies for teaching and using molecular simulation. Fluid Phase Equilibria, 2002, 194-197, 327-335.	1.4	18
126	Accuracy of free-energy perturbation calculations in molecular simulation. II. Heuristics. Journal of Chemical Physics, 2001, 115, 6866-6875.	1.2	89

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127	Accuracy of free-energy perturbation calculations in molecular simulation. I. Modeling. Journal of Chemical Physics, 2001, 114, 7303-7311.	1.2	135
128	A general-purpose biasing scheme for Monte Carlo simulation of associating fluids. Journal of Chemical Physics, 2001, 114, 8752-8762.	1.2	42
129	Exact solution for the singlet density distributions and second-order correlations of normal-mode coordinates for hard rods in one dimension. Journal of Chemical Physics, 1999, 110, 11390-11398.	1.2	5
130	Freezing of polydisperse hard spheres. Physical Review E, 1999, 59, 618-622.	0.8	152
131	Optimal intermediates in staged free energy calculations. Journal of Chemical Physics, 1999, 111, 4414-4423.	1.2	52
132	A comparison of molecular-based models to determine vaporâ€“liquid phase coexistence in hydrogen fluoride. Fluid Phase Equilibria, 1999, 158-160, 37-47.	1.4	27
133	Evaluation of a locus of azeotropes by molecular simulation. AICHE Journal, 1999, 45, 2237-2244.	1.8	11
134	Modeling the Monte Carlo simulation of associating fluids. Journal of Chemical Physics, 1999, 110, 5493-5502.	1.2	17
135	Improved Thermodynamic Equation of State for Hydrogen Fluoride. Industrial & Engineering Chemistry Research, 1999, 38, 4125-4129.	1.8	21
136	Thermodynamic Integration Along Coexistence Lines. Theoretical and Computational Chemistry, 1999, 7, 99-127.	0.2	2
137	Precision and accuracy of staged free-energy perturbation methods for computing the chemical potential by molecular simulation. Fluid Phase Equilibria, 1998, 150-151, 41-49.	1.4	80
138	Vaporâ€“liquid equilibria and heat effects of hydrogen fluoride from molecular simulation. Journal of Chemical Physics, 1998, 109, 4015-4027.	1.2	23
139	Quantitative comparison and optimization of methods for evaluating the chemical potential by molecular simulation. Molecular Physics, 1997, 92, 973-996.	0.8	175
140	Perturbation solution to the convectionâ€“diffusion equation with moving fronts. AICHE Journal, 1997, 43, 631-644.	1.8	3
141	Potential for use of liquid crystals as dynamically tunable electrophoretic media. AICHE Journal, 1997, 43, 1366-1368.	1.8	2
142	Thermal properties of hydrogen fluoride from EOS+ association model. AICHE Journal, 1997, 43, 2381-2384.	1.8	12
143	Tracer diffusion in perfectly aligned liquid crystalline phases Kinetic theory and molecular dynamics simulations. Molecular Physics, 1997, 91, 993-1004.	0.8	3
144	Convection-diffusion of solutes in media with piecewise constant transport properties. Chemical Engineering Science, 1996, 51, 5299-5312.	1.9	6

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145	Simulation of adsorption of liquid mixtures of N2 and O2 in a model faujasite cavity at 77.5 K. Adsorption, 1996, 2, 41-50.	1.4	17
146	The isotropicâ€“nematic phase transition in uniaxial hard ellipsoid fluids: Coexistence data and the approach to the Onsager limit. Journal of Chemical Physics, 1996, 105, 2837-2849.	1.2	116
147	Monte Carlo study of freezing of polydisperse hard spheres. Physical Review E, 1996, 54, 634-643.	0.8	173
148	Numerical study of freezing in polydisperse colloidal suspensions. Journal of Physics Condensed Matter, 1996, 8, 9627-9631.	0.7	14
149	Transformation and topological reduction of cluster expansions usingm-bonds. Journal of Statistical Physics, 1995, 78, 877-892.	0.5	1
150	Thermodynamic and structural properties of model systems at solid-fluid coexistence. Molecular Physics, 1995, 85, 23-42.	0.8	177
151	A theory for the 1â€1/2 fluid. Journal of Chemical Physics, 1995, 103, 1599-1606.	1.2	3
152	Molecular simulation in a pseudo grand canonical ensemble. Molecular Physics, 1995, 86, 139-147.	0.8	37
153	Thermodynamic and structural properties of model systems at solid-fluid coexistence. Molecular Physics, 1995, 85, 43-59.	0.8	278
154	Solid-Fluid Coexistence for Inverse-Power Potentials. Physical Review Letters, 1995, 74, 122-125.	2.9	130
155	Efficient evaluation of three-phase coexistence lines. International Journal of Thermophysics, 1994, 15, 1073-1083.	1.0	16
156	Coexistence diagrams of mixtures by molecular simulation. Chemical Engineering Science, 1994, 49, 2633-2645.	1.9	125
157	Self-diffusion in the nematic and smectic A phases of an aligned fluid of hard spherocylinders. Molecular Physics, 1994, 83, 101-112.	0.8	5
158	Gibbs-Duhem integration: a new method for direct evaluation of phase coexistence by molecular simulation. Molecular Physics, 1993, 78, 1331-1336.	0.8	324
159	Direct evaluation of phase coexistence by molecular simulation via integration along the saturation line. Journal of Chemical Physics, 1993, 98, 4149-4162.	1.2	568
160	Implementation of the Gibbs ensemble using a thermodynamic model for one of the coexisting phases. Molecular Physics, 1993, 79, 39-52.	0.8	13
161	Hard particles in narrow pores. Transferâ€matrix solution and the periodic narrow box. Journal of Chemical Physics, 1993, 98, 4853-4861.	1.2	46
162	Fluids confined to narrow pores: A low-dimensional approach. Physical Review A, 1992, 45, 939-952.	1.0	18

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163	Oneâ€andâ€aâ€halfâ€fluid theory: A new approach to conformal solutions. Journal of Chemical Physics, 1991, 95, 7518-7525.	1.2	1
164	Solid-Fluid Coexistence in Binary Hard Sphere Mixtures by Semigrand Monte Carlo Simulation. Molecular Simulation, 1991, 7, 285-302.	0.9	49
165	Conserving energy during molecular dynamics simulations of water, proteins, and proteins in water. Journal of Computational Chemistry, 1990, 11, 1169-1180.	1.5	86
166	A composition density functional theory for mixtures based upon an infinitely polydisperse reference. II. Freezing in hard sphere mixtures. Journal of Chemical Physics, 1990, 92, 4417-4425.	1.2	3
167	A composition density functional theory for mixtures based upon an infinitely polydisperse reference. I. Formalism and theory. Journal of Chemical Physics, 1990, 92, 658-666.	1.2	5
168	Infinitely polydisperse fluids. Journal of Chemical Physics, 1989, 90, 439-447.	1.2	31
169	Monte Carlo simulation of multicomponent equilibria in a semigrand canonical ensemble. Molecular Physics, 1988, 64, 1105-1131.	0.8	233
170	An efficient algorithm for the computation of pair correlation functions for hard spheres in the Percus-Yevick theory. Molecular Physics, 1988, 64, 125-128.	0.8	10
171	Nearly monodisperse fluids. I. Monte Carlo simulations of Lennardâ€Jones particles in a semigrand ensemble. Journal of Chemical Physics, 1987, 87, 4881-4890.	1.2	68
172	Monte carlo simulation of continuous Lennard-Jones mixtures. Fluid Phase Equilibria, 1986, 29, 327-335.	1.4	13