

David A Kofke

List of Publications by Year in descending order

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172
papers

6,932
citations

71102

41
h-index

66911

78
g-index

180
all docs

180
docs citations

180
times ranked

3166
citing authors

#	ARTICLE	IF	CITATIONS
1	Direct evaluation of phase coexistence by molecular simulation via integration along the saturation line. <i>Journal of Chemical Physics</i> , 1993, 98, 4149-4162.	3.0	568
2	Gibbs-Duhem integration: a new method for direct evaluation of phase coexistence by molecular simulation. <i>Molecular Physics</i> , 1993, 78, 1331-1336.	1.7	324
3	Thermodynamic and structural properties of model systems at solid-fluid coexistence. <i>Molecular Physics</i> , 1995, 85, 43-59.	1.7	278
4	Monte Carlo simulation of multicomponent equilibria in a semigrand canonical ensemble. <i>Molecular Physics</i> , 1988, 64, 1105-1131.	1.7	233
5	On the acceptance probability of replica-exchange Monte Carlo trials. <i>Journal of Chemical Physics</i> , 2002, 117, 6911-6914.	3.0	200
6	Thermodynamic and structural properties of model systems at solid-fluid coexistence. <i>Molecular Physics</i> , 1995, 85, 23-42.	1.7	177
7	Quantitative comparison and optimization of methods for evaluating the chemical potential by molecular simulation. <i>Molecular Physics</i> , 1997, 92, 973-996.	1.7	175
8	Appropriate methods to combine forward and reverse free-energy perturbation averages. <i>Journal of Chemical Physics</i> , 2003, 118, 2977-2984.	3.0	174
9	Monte Carlo study of freezing of polydisperse hard spheres. <i>Physical Review E</i> , 1996, 54, 634-643.	2.1	173
10	Mayer Sampling: Calculation of Cluster Integrals using Free-Energy Perturbation Methods. <i>Physical Review Letters</i> , 2004, 92, 220601.	7.8	156
11	Freezing of polydisperse hard spheres. <i>Physical Review E</i> , 1999, 59, 618-622.	2.1	152
12	Improving the efficiency and reliability of free energy perturbation calculations using overlap sampling methods. <i>Journal of Computational Chemistry</i> , 2004, 25, 28-40.	3.3	145
13	Selection of temperature intervals for parallel-tempering simulations. <i>Journal of Chemical Physics</i> , 2005, 122, 206101.	3.0	136
14	Accuracy of free-energy perturbation calculations in molecular simulation. I. Modeling. <i>Journal of Chemical Physics</i> , 2001, 114, 7303-7311.	3.0	135
15	Surface tension and vapor-liquid phase coexistence of the square-well fluid. <i>Journal of Chemical Physics</i> , 2003, 119, 3405-3412.	3.0	134
16	Phase-space overlap measures. I. Fail-safe bias detection in free energies calculated by molecular simulation. <i>Journal of Chemical Physics</i> , 2005, 123, 054103.	3.0	131
17	Solid-Fluid Coexistence for Inverse-Power Potentials. <i>Physical Review Letters</i> , 1995, 74, 122-125.	7.8	130
18	Coexistence diagrams of mixtures by molecular simulation. <i>Chemical Engineering Science</i> , 1994, 49, 2633-2645.	3.8	125

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19	The isotropic-nematic phase transition in uniaxial hard ellipsoid fluids: Coexistence data and the approach to the Onsager limit. <i>Journal of Chemical Physics</i> , 1996, 105, 2837-2849.	3.0	116
20	Calculation of surface tension via area sampling. <i>Journal of Chemical Physics</i> , 2007, 127, 174709.	3.0	99
21	Phase-space overlap measures. II. Design and implementation of staging methods for free-energy calculations. <i>Journal of Chemical Physics</i> , 2005, 123, 084109.	3.0	95
22	Accuracy of free-energy perturbation calculations in molecular simulation. II. Heuristics. <i>Journal of Chemical Physics</i> , 2001, 115, 6866-6875.	3.0	89
23	Free energy methods in molecular simulation. <i>Fluid Phase Equilibria</i> , 2005, 228-229, 41-48.	2.5	87
24	Conserving energy during molecular dynamics simulations of water, proteins, and proteins in water. <i>Journal of Computational Chemistry</i> , 1990, 11, 1169-1180.	3.3	86
25	Precision and accuracy of staged free-energy perturbation methods for computing the chemical potential by molecular simulation. <i>Fluid Phase Equilibria</i> , 1998, 150-151, 41-49.	2.5	80
26	Higher-Order Virial Coefficients of Water Models. <i>Journal of Physical Chemistry B</i> , 2007, 111, 11463-11473.	2.6	78
27	Nearly monodisperse fluids. I. Monte Carlo simulations of Lennard-Jones particles in a semigrand ensemble. <i>Journal of Chemical Physics</i> , 1987, 87, 4881-4890.	3.0	68
28	Sixth, seventh and eighth virial coefficients of the Lennard-Jones model. <i>Molecular Physics</i> , 2009, 107, 2309-2318.	1.7	66
29	Fifth to eleventh virial coefficients of hard spheres. <i>Physical Review E</i> , 2014, 90, 023301.	2.1	59
30	Optimal intermediates in staged free energy calculations. <i>Journal of Chemical Physics</i> , 1999, 111, 4414-4423.	3.0	52
31	Fourth and Fifth Virial Coefficients of Polarizable Water. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7810-7815.	2.6	51
32	Virial Coefficients of Polarizable Water: Applications to Thermodynamic Properties and Molecular Clustering. <i>Journal of Physical Chemistry C</i> , 2007, 111, 16021-16027.	3.1	50
33	Solid-Fluid Coexistence in Binary Hard Sphere Mixtures by Semigrand Monte Carlo Simulation. <i>Molecular Simulation</i> , 1991, 7, 285-302.	2.0	49
34	Improved models for the phase behaviour of hydrogen fluoride: chain and ring aggregates in the SAFT approach and the AEOS model. <i>Molecular Physics</i> , 2002, 100, 2241-2259.	1.7	49
35	Getting the most from molecular simulation. <i>Molecular Physics</i> , 2004, 102, 405-420.	1.7	49
36	Hard particles in narrow pores. Transfer-matrix solution and the periodic narrow box. <i>Journal of Chemical Physics</i> , 1993, 98, 4853-4861.	3.0	46

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37	Staging Is More Important than Perturbation Method for Computation of Enthalpy and Entropy Changes in Complex Systems. <i>Journal of Physical Chemistry B</i> , 2003, 107, 5598-5611.	2.6	45
38	Rosenbluth-sampled nonequilibrium work method for calculation of free energies in molecular simulation. <i>Journal of Chemical Physics</i> , 2005, 122, 204104.	3.0	45
39	Model for small-sample bias of free-energy calculations applied to Gaussian-distributed nonequilibrium work measurements. <i>Journal of Chemical Physics</i> , 2004, 121, 8742-8747.	3.0	44
40	Atomistic modeling of β -Sn surface energies and adatom diffusivity. <i>Applied Surface Science</i> , 2010, 256, 4402-4407.	6.1	44
41	Gas-Phase Molecular Clustering of TIP4P and SPC/E Water Models from Higher-Order Virial Coefficients. <i>Industrial & Engineering Chemistry Research</i> , 2006, 45, 5566-5573.	3.7	43
42	Comprehensive high-precision high-accuracy equation of state and coexistence properties for classical Lennard-Jones crystals and low-temperature fluid phases. <i>Journal of Chemical Physics</i> , 2018, 149, 204508.	3.0	43
43	A general-purpose biasing scheme for Monte Carlo simulation of associating fluids. <i>Journal of Chemical Physics</i> , 2001, 114, 8752-8762.	3.0	42
44	Path-integral Mayer-sampling calculations of the quantum Boltzmann contribution to virial coefficients of helium-4. <i>Journal of Chemical Physics</i> , 2012, 137, 184101.	3.0	42
45	Lattice Strain Due to an Atomic Vacancy. <i>International Journal of Molecular Sciences</i> , 2009, 10, 2798-2808.	4.1	40
46	Virial coefficients of model alkanes. <i>Journal of Chemical Physics</i> , 2010, 133, 104101.	3.0	40
47	Semigrand Canonical Monte Carlo Simulation; Integration Along Coexistence Lines. <i>Advances in Chemical Physics</i> , 2007, , 405-441.	0.3	39
48	Molecular simulation in a pseudo grand canonical ensemble. <i>Molecular Physics</i> , 1995, 86, 139-147.	1.7	37
49	Using overlap and funnel sampling to obtain accurate free energies from nonequilibrium work measurements. <i>Physical Review E</i> , 2004, 69, 057702.	2.1	37
50	Comment on "The incomplete beta function law for parallel tempering sampling of classical canonical systems" [J. Chem. Phys. 120, 4119 (2004)]. <i>Journal of Chemical Physics</i> , 2004, 121, 1167-1167.	3.0	36
51	Molecular simulation study of miscibility of ternary and quaternary InGaAlN alloys. <i>Journal of Applied Physics</i> , 2004, 95, 6129-6137.	2.5	35
52	$\langle mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"> \langle mml:mrow> \langle mml:mi> \hat{I}^2 \langle /mml:mi> \langle mml:mtext> -Sn \langle /mml:mtext> \langle /mml:mrow> \langle /mml:math>$ grain boundary structure and self-diffusivity via molecular dynamics simulations. <i>Physical Review B</i> , 2010, 81, .	3.0	35
53	Eighth to sixteenth virial coefficients of the Lennard-Jones model. <i>Journal of Chemical Physics</i> , 2015, 143, 044504.	3.0	33
54	On the sampling requirements for exponential-work free-energy calculations. <i>Molecular Physics</i> , 2006, 104, 3701-3708.	1.7	32

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55	Infinitely polydisperse fluids. <i>Journal of Chemical Physics</i> , 1989, 90, 439-447.	3.0	31
56	Molecular simulation study of miscibility in $\text{In}_x\text{Ga}_{1-x}\text{N}$ ternary alloys. <i>Journal of Applied Physics</i> , 2004, 95, 4500-4502.	2.5	30
57	Asymmetric bias in free-energy perturbation measurements using two Hamiltonian-based models. <i>Physical Review E</i> , 2004, 70, 066702.	2.1	30
58	Molecular simulation study of effect of molecular association on vapor-liquid interfacial properties. <i>Journal of Chemical Physics</i> , 2004, 121, 9574-9580.	3.0	30
59	Semiclassical fifth virial coefficients for improved ab initio helium-4 standards. <i>Chemical Physics Letters</i> , 2012, 531, 11-17.	2.6	28
60	Mayer Sampling Monte Carlo calculation of virial coefficients on graphics processors. <i>Molecular Physics</i> , 2013, 111, 535-543.	1.7	28
61	A comparison of molecular-based models to determine vapor-liquid phase coexistence in hydrogen fluoride. <i>Fluid Phase Equilibria</i> , 1999, 158-160, 37-47.	2.5	27
62	Mayer-sampling Monte Carlo calculations of uniquely flexible contributions to virial coefficients. <i>Journal of Chemical Physics</i> , 2011, 135, 124101.	3.0	27
63	Very fast averaging of thermal properties of crystals by molecular simulation. <i>Physical Review E</i> , 2015, 92, 043303.	2.1	27
64	Hydrogen fluoride phase behavior and molecular structure: A QM/MM potential model approach. <i>Journal of Chemical Physics</i> , 2003, 119, 7365-7371.	3.0	26
65	Accurate and precise <i>ab initio</i> anharmonic free-energy calculations for metallic crystals: Application to hcp Fe at high temperature and pressure. <i>Physical Review B</i> , 2017, 96, .	3.2	25
66	Reformulation of Ensemble Averages via Coordinate Mapping. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1491-1498.	5.3	24
67	Vapor-liquid equilibria and heat effects of hydrogen fluoride from molecular simulation. <i>Journal of Chemical Physics</i> , 1998, 109, 4015-4027.	3.0	23
68	Quantifying Computational Effort Required for Stochastic Averages. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5229-5234.	5.3	23
69	<i>Etomica</i> : An object-oriented framework for molecular simulation. <i>Journal of Computational Chemistry</i> , 2015, 36, 573-583.	3.3	22
70	Improved Thermodynamic Equation of State for Hydrogen Fluoride. <i>Industrial & Engineering Chemistry Research</i> , 1999, 38, 4125-4129.	3.7	21
71	Molecular Simulation Study of the Vapor-Liquid Interfacial Behavior of a Dimer-forming Associating Fluid. <i>Molecular Simulation</i> , 2004, 30, 343-351.	2.0	21
72	Efficient calculation of temperature dependence of solid-phase free energies by overlap sampling coupled with harmonically targeted perturbation. <i>Journal of Chemical Physics</i> , 2010, 133, 134104.	3.0	21

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73	Virial coefficients, equation of state, and solid–fluid coexistence for the soft sphere model. <i>Molecular Physics</i> , 2011, 109, 123-132.	1.7	21
74	Communication: Analytic continuation of the virial series through the critical point using parametric approximants. <i>Journal of Chemical Physics</i> , 2015, 143, 071103.	3.0	21
75	The effect of truncation and shift on virial coefficients of Lennard–Jones potentials. <i>Collection of Czechoslovak Chemical Communications</i> , 2010, 75, 447-462.	1.0	21
76	Vapor-phase metastability and condensation via the virial equation of state with extrapolated coefficients. <i>Fluid Phase Equilibria</i> , 2016, 409, 12-18.	2.5	20
77	Harmonically Assisted Methods for Computing the Free Energy of Classical Crystals by Molecular Simulation: A Comparative Study. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 825-834.	5.3	20
78	Suitability of umbrella- and overlap-sampling methods for calculation of solid-phase free energies by molecular simulation. <i>Journal of Chemical Physics</i> , 2010, 132, 214103.	3.0	19
79	Calculation of inhomogeneous-fluid cluster expansions with application to the hard-sphere/hard-wall system. <i>Journal of Chemical Physics</i> , 2013, 138, 134706.	3.0	19
80	Critical isotherms from virial series using asymptotically consistent approximants. <i>AIChE Journal</i> , 2014, 60, 3336-3349.	3.6	19
81	Virial Coefficients and Equations of State for Hard Polyhedron Fluids. <i>Langmuir</i> , 2017, 33, 11788-11796.	3.5	19
82	Fluids confined to narrow pores: A low-dimensional approach. <i>Physical Review A</i> , 1992, 45, 939-952.	2.5	18
83	Web-based technologies for teaching and using molecular simulation. <i>Fluid Phase Equilibria</i> , 2002, 194-197, 327-335.	2.5	18
84	Effect of Cu and Ag solute segregation on $\langle i \rangle^2 \langle i \rangle$ Sn grain boundary diffusivity. <i>Journal of Applied Physics</i> , 2011, 110, 013528.	2.5	18
85	A comparative study of methods to compute the free energy of an ordered assembly by molecular simulation. <i>Journal of Chemical Physics</i> , 2013, 139, 084105.	3.0	18
86	Simulation of adsorption of liquid mixtures of N ₂ and O ₂ in a model faujasite cavity at 77.5 K. <i>Adsorption</i> , 1996, 2, 41-50.	3.0	17
87	Modeling the Monte Carlo simulation of associating fluids. <i>Journal of Chemical Physics</i> , 1999, 110, 5493-5502.	3.0	17
88	Hydrogen fluoride phase behavior and molecular structure: Ab initio derived potential models. <i>Journal of Chemical Physics</i> , 2003, 119, 6092-6099.	3.0	17
89	Virial Coefficients of Helium-4 from $\langle i \rangle$ Ab Initio $\langle i \rangle$ -Based Molecular Models. <i>Journal of Chemical & Engineering Data</i> , 2019, 64, 3742-3754.	1.9	17
90	Efficient evaluation of three-phase coexistence lines. <i>International Journal of Thermophysics</i> , 1994, 15, 1073-1083.	2.1	16

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91	Evaluation of bridge-function diagrams via Mayer-sampling Monte Carlo simulation. Journal of Chemical Physics, 2005, 122, 104508.	3.0	16
92	Effects of thermostating in molecular dynamics on anharmonic properties of crystals: Application to fcc Al at high pressure and temperature. Journal of Chemical Physics, 2018, 149, 124109.	3.0	16
93	Integral-equation theories and Mayer-sampling Monte Carlo: a tandem approach for computing virial coefficients of simple fluids. Molecular Physics, 2011, 109, 2395-2406.	1.7	15
94	Molecular-based virial coefficients of CO ₂ -H ₂ O mixtures. AIChE Journal, 2015, 61, 3029-3037.	3.6	15
95	Force-sampling methods for density distributions as instances of mapped averaging. Molecular Physics, 2019, 117, 2822-2829.	1.7	15
96	Numerical study of freezing in polydisperse colloidal suspensions. Journal of Physics Condensed Matter, 1996, 8, 9627-9631.	1.8	14
97	Monte Carlo and cell model calculations for the solid-fluid phase behaviour of the triangle-well model. Molecular Physics, 2002, 100, 1543-1550.	1.7	14
98	Variational formula for the free energy based on incomplete sampling in a molecular simulation. Physical Review E, 2003, 68, 026122.	2.1	14
99	Virial coefficients of Lennard-Jones mixtures. Journal of Chemical Physics, 2009, 130, 224104.	3.0	14
100	Monte carlo simulation of continuous Lennard-Jones mixtures. Fluid Phase Equilibria, 1986, 29, 327-335.	2.5	13
101	Implementation of the Gibbs ensemble using a thermodynamic model for one of the coexisting phases. Molecular Physics, 1993, 79, 39-52.	1.7	13
102	Combined temperature and density series for fluid-phase properties. II. Lennard-Jones spheres. Journal of Chemical Physics, 2019, 151, 204501.	3.0	13
103	Thermal properties of hydrogen fluoride from EOS+ association model. AIChE Journal, 1997, 43, 2381-2384.	3.6	12
104	Combined temperature and density series for fluid-phase properties. I. Square-well spheres. Journal of Chemical Physics, 2015, 143, 114110.	3.0	12
105	Evaluation of a locus of azeotropes by molecular simulation. AIChE Journal, 1999, 45, 2237-2244.	3.6	11
106	Fugacity Coefficients of Saturated Water from Molecular Simulation. Journal of Physical Chemistry B, 2003, 107, 12808-12813.	2.6	11
107	Alternatives to conventional ensemble averages for thermodynamic properties. Current Opinion in Chemical Engineering, 2019, 23, 70-76.	7.8	11
108	An efficient algorithm for the computation of pair correlation functions for hard spheres in the Percus-Yevick theory. Molecular Physics, 1988, 64, 125-128.	1.7	10

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109	Interpolation of virial coefficients. <i>Molecular Physics</i> , 2009, 107, 1431-1436.	1.7	10
110	Modeling solubility in supercritical fluids via the virial equation of state. <i>Journal of Supercritical Fluids</i> , 2010, 55, 479-484.	3.2	10
111	Second through fifth virial coefficients for model methane-ethane mixtures. <i>Fluid Phase Equilibria</i> , 2013, 351, 69-73.	2.5	10
112	Molecular Simulation Study of the Effect of Pressure on the Vapor-Liquid Interface of the Square-Well Fluid. <i>Langmuir</i> , 2005, 21, 4218-4226.	3.5	9
113	Solute Effects on $\hat{\Gamma}^2$ -Sn Grain Boundary Energy and Shear Stress. <i>Journal of Nanomechanics & Micromechanics</i> , 2011, 1, 41-50.	1.4	9
114	Efficient calculation of $\langle i \rangle^{\pm}$ - and $\langle i \rangle^2$ -nitrogen free energies and coexistence conditions via overlap sampling with targeted perturbation. <i>Journal of Chemical Physics</i> , 2011, 135, 044125.	3.0	9
115	Virial Equation of State of Water Based on Wertheim's Association Theory. <i>Journal of Physical Chemistry B</i> , 2012, 116, 14078-14088.	2.6	9
116	Thermodynamic Properties of Supercritical CO ₂ /CH ₄ Mixtures from the Virial Equation of State. <i>Journal of Chemical & Engineering Data</i> , 2016, 61, 4296-4312.	1.9	9
117	Free energy and concentration of crystalline vacancies by molecular simulation. <i>Molecular Physics</i> , 2018, 116, 3027-3041.	1.7	9
118	Cluster integrals and virial coefficients for realistic molecular models. <i>Physical Review E</i> , 2020, 101, 051301.	2.1	9
119	Self-referential method for calculation of the free energy of crystals by Monte Carlo simulation. <i>Physical Review E</i> , 2002, 65, 036709.	2.1	8
120	UB association bias algorithm applied to the simulation of hydrogen fluoride. <i>Fluid Phase Equilibria</i> , 2002, 194-197, 249-256.	2.5	8
121	Elastic constants and the effect of strain on monovacancy concentration in fcc hard-sphere crystals. <i>Physical Review B</i> , 2004, 70, .	3.2	8
122	The rate of convergence of the virial series in confined systems. <i>Molecular Physics</i> , 2015, 113, 1179-1189.	1.7	8
123	Calculation of high-order virial coefficients for the square-well potential. <i>Physical Review E</i> , 2016, 94, 013301.	2.1	8
124	Speed of Sound in Helium-4 from Ab Initio Acoustic Virial Coefficients. <i>Journal of Chemical & Engineering Data</i> , 2021, 66, 3258-3281.	1.9	8
125	Three-body effects in hydrogen fluoride: survey of potential energy surfaces. <i>Molecular Physics</i> , 2006, 104, 503-513.	1.7	7
126	Mayer-sampling Monte Carlo calculations of methanol virial coefficients. <i>Molecular Simulation</i> , 2010, 36, 1282-1288.	2.0	7

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127	Interpreting Gas-Saturation Vapor-Pressure Measurements Using Virial Coefficients Derived from Molecular Models. <i>Journal of Chemical & Engineering Data</i> , 2014, 59, 3183-3192.	1.9	7
128	Evaluation of second and third dielectric virial coefficients for non-polarisable molecular models. <i>Molecular Physics</i> , 2017, 115, 991-1003.	1.7	7
129	No system-size anomalies in entropy of bcc iron at Earth's inner-core conditions. <i>Scientific Reports</i> , 2018, 8, 7295.	3.3	7
130	Convection-diffusion of solutes in media with piecewise constant transport properties. <i>Chemical Engineering Science</i> , 1996, 51, 5299-5312.	3.8	6
131	Effect of monovacancies on the relative stability of fcc and hcp hard-sphere crystals. <i>Journal of Chemical Physics</i> , 2005, 122, 176101.	3.0	6
132	Algorithm for constant-pressure Monte Carlo simulation of crystalline solids. <i>Physical Review E</i> , 2011, 84, 046712.	2.1	6
133	Effects of Finite Size and Proton Disorder on Lattice-Dynamics Estimates of the Free Energy of Clathrate Hydrates. <i>Industrial & Engineering Chemistry Research</i> , 2015, 54, 4487-4496.	3.7	6
134	Quantum virial coefficients of molecular nitrogen. <i>Molecular Physics</i> , 2017, 115, 869-878.	1.7	6
135	Molecular Calculation of the Critical Parameters of Classical Helium. <i>Journal of Chemical & Engineering Data</i> , 2020, 65, 1028-1037.	1.9	6
136	A composition density functional theory for mixtures based upon an infinitely polydisperse reference. I. Formalism and theory. <i>Journal of Chemical Physics</i> , 1990, 92, 658-666.	3.0	5
137	Self-diffusion in the nematic and smectic A phases of an aligned fluid of hard spherocylinders. <i>Molecular Physics</i> , 1994, 83, 101-112.	1.7	5
138	Exact solution for the singlet density distributions and second-order correlations of normal-mode coordinates for hard rods in one dimension. <i>Journal of Chemical Physics</i> , 1999, 110, 11390-11398.	3.0	5
139	Trimer Based Polarization as a Multibody Molecular Model. Application to Hydrogen Fluoride. <i>Journal of the American Chemical Society</i> , 2005, 127, 690-698.	13.7	5
140	Molecular Based Modeling of Associating Fluids via Calculation of Wertheim Cluster Integrals. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11515-11524.	2.6	5
141	Perspective: Free Energies and Phase Equilibria. , 2005, , 683-705.		5
142	Liquid-Phase Activity Coefficients for Saturated HF/H ₂ O Mixtures with Vapor-Phase Nonidealities Described by Molecular Simulation. <i>Industrial & Engineering Chemistry Research</i> , 2004, 43, 218-227.	3.7	4
143	Direct orientation sampling of diatomic molecules for path integral Monte Carlo calculation of fully quantum virial coefficients. <i>Journal of Chemical Physics</i> , 2017, 146, .	3.0	4
144	Highlighting 10 Years of NIST Cooperation and Service to the Thermophysical Properties Data Community. <i>Journal of Chemical & Engineering Data</i> , 2019, 64, 4191-4192.	1.9	4

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145	Alternative ensemble averages in molecular dynamics simulation of hard spheres. <i>Molecular Physics</i> , 2019, 117, 3734-3753.	1.7	4
146	Identifying and estimating bias in overlap-sampling free-energy calculations. <i>Molecular Simulation</i> , 2021, 47, 379-389.	2.0	4
147	pyHMA: A VASP post-processor for precise measurement of crystalline anharmonic properties using harmonically mapped averaging. <i>Computer Physics Communications</i> , 2021, 258, 107554.	7.5	4
148	A composition density functional theory for mixtures based upon an infinitely polydisperse reference. II. Freezing in hard sphere mixtures. <i>Journal of Chemical Physics</i> , 1990, 92, 4417-4425.	3.0	3
149	A theory for the $1\frac{1}{2}$ fluid. <i>Journal of Chemical Physics</i> , 1995, 103, 1599-1606.	3.0	3
150	Perturbation solution to the convection-diffusion equation with moving fronts. <i>AIChE Journal</i> , 1997, 43, 631-644.	3.6	3
151	A comparison of some variational formulas for the free energy as applied to hard-sphere crystals. <i>Journal of Chemical Physics</i> , 2002, 117, 9111-9115.	3.0	3
152	Free-energy calculations for fluid and solid phases by molecular simulation. <i>Fluid Phase Equilibria</i> , 2002, 194-197, 219-226.	2.5	3
153	Implementation of harmonically mapped averaging in LAMMPS, and effect of potential truncation on anharmonic properties. <i>Journal of Chemical Physics</i> , 2020, 152, 014107.	3.0	3
154	Properties of supercritical N ₂ , O ₂ , CO ₂ , and NH ₃ mixtures from the virial equation of state. <i>AIChE Journal</i> , 2021, 67, e17072.	3.6	3
155	Tracer diffusion in perfectly aligned liquid crystalline phases Kinetic theory and molecular dynamics simulations. <i>Molecular Physics</i> , 1997, 91, 993-1004.	1.7	3
156	Potential for use of liquid crystals as dynamically tunable electrophoretic media. <i>AIChE Journal</i> , 1997, 43, 1366-1368.	3.6	2
157	Thermodynamic Integration Along Coexistence Lines. <i>Theoretical and Computational Chemistry</i> , 1999, 7, 99-127.	0.4	2
158	Electric-field mapped averaging for the dielectric constant. <i>Fluid Phase Equilibria</i> , 2018, 470, 17-24.	2.5	2
159	One-dimensional fluid theory: A new approach to conformal solutions. <i>Journal of Chemical Physics</i> , 1991, 95, 7518-7525.	3.0	1
160	Transformation and topological reduction of cluster expansions using m-bonds. <i>Journal of Statistical Physics</i> , 1995, 78, 877-892.	1.2	1
161	Peer Review Appreciation at JCED. <i>Journal of Chemical & Engineering Data</i> , 2018, 63, 3169-3169.	1.9	1
162	Introducing JCED's Latin America Special Issue. <i>Journal of Chemical & Engineering Data</i> , 2019, 64, 1859-1859.	1.9	1

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163	Historical Perspective of the Journal of Chemical & Engineering Data's Published Topics, 1956-2020. Journal of Chemical & Engineering Data, 2021, 66, 1555-1556.	1.9	1
164	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.	2.6	1
165	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.	1.9	1
166	Perspective: Free Energies and Phase Equilibria. , 2005, , 683-705.		1
167	Solder joint grain boundary structure and diffusivity via molecular dynamics simulations. , 2012, , .		0
168	Mixed-precision models for calculation of high-order virial coefficients on GPUs. , 2014, , .		0
169	Quantum Virial Coefficients via Path Integral Monte Carlo with Semi-classical Beads. Molecular Modeling and Simulation, 2016, , 93-106.	0.2	0
170	Journal of Chemical & Engineering Data: An Update from the Editorial Team. Journal of Chemical & Engineering Data, 2021, 66, 1-2.	1.9	0
171	Journal of Chemical & Engineering Data: Why Change the Cover Page?. Journal of Chemical & Engineering Data, 2021, 66, 859-860.	1.9	0
172	Molecular Calculation of the Critical Parameters of Classical Helium. Journal of Chemical & Engineering Data, 2019, 65, .	1.9	0