Jeffrey R Errington

List of Publications by Year
in descending order

105	6,571	61857	64668
papers	citations	43 h-index	79 g-index

109	109	109	3729
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Relationship between structural order and the anomalies of liquid water. Nature, 2001, 409, 318-321.	13.7	1,320
2	Direct calculation of liquidâ€“vapor phase equilibria from transition matrix Monte Carlo simulation. Journal of Chemical Physics, 2003, 118, 9915-9925.	1.2	262
3	A Fixed Point Charge Model for Water Optimized to the Vaporâˆ’Liquid Coexistence Properties. Journal of Physical Chemistry B, 1998, 102, 7470-7475.	1.2	178
4	A New Intermolecular Potential Model for the n-Alkane Homologous Series. Journal of Physical Chemistry B, 1999, 103, 6314-6322.	1.2	171
5	A computational study of hydration, solution structure, and dynamics in dilute carbohydrate solutions. Journal of Chemical Physics, 2005, 122, 204511.	1.2	166
6	Layering and Position-Dependent Diffusive Dynamics of Confined Fluids. Physical Review Letters, 2008, 100, 145901.	2.9	161
7	Evaluating surface tension using grand-canonical transition-matrix Monte Carlo simulation and finite-size scaling. Physical Review E, 2003, 67, 012102.	0.8	154
8	Excess-entropy-based anomalies for a waterlike fluid. Journal of Chemical Physics, 2006, 125, 244502.	1.2	148
9	Surface tension and vaporâ€“liquid phase coexistence of the square-well fluid. Journal of Chemical Physics, 2003, 119, 3405-3412.	1.2	134
10	Thermodynamics Predicts How Confinement Modifies the Dynamics of the Equilibrium Hard-Sphere Fluid. Physical Review Letters, 2006, 96, 177804.	2.9	133
11	Quantification of order in the Lennard-Jones system. Journal of Chemical Physics, 2003, 118, 2256-2263.	1.2	124
12	Nucleation and cavitation of spherical, cylindrical, and slablike droplets and bubbles in small systems. Journal of Chemical Physics, 2006, 125, 034705.	1.2	123
13	Molecular Simulation of Phase Equilibria for Waterâˆ’Methane and Waterâˆ’Ethane Mixtures. Journal of Physical Chemistry B, 1998, 102, 8865-8873.	1.2	115
14	New intermolecular potential models for benzene and cyclohexane. Journal of Chemical Physics, 1999, 111, 9731-9738.	1.2	113
15	Relationship between thermodynamics and dynamics of supercooled liquids. Journal of Chemical Physics, 2006, 125, 076102.	1.2	106
16	Cooperative Origin of Low-Density Domains in Liquid Water. Physical Review Letters, 2002, 89, 215503.	2.9	103
17	Anomalous structure and dynamics of the Gaussian-core fluid. Physical Review E, 2009, 79, 031203.	0.8	100
18	Calculation of surface tension via area sampling. Journal of Chemical Physics, 2007, 127, 174709.	1.2	99

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19	Phase equilibria of the modified Buckingham exponential-6 potential from Hamiltonian scaling grand canonical Monte Carlo. Journal of Chemical Physics, 1998, 109, 1093-1100.	1.2	98
20	Quantitative Link between Single-Particle Dynamics and Static Structure of Supercooled Liquids. Journal of Physical Chemistry B, 2006, 110, 18147-18150.	1.2	95
21	Relationships between Self-Diffusivity, Packing Fraction, and Excess Entropy in Simple Bulk and Confined Fluids. Journal of Physical Chemistry B, 2007, 111, 10054-10063.	1.2	94
22	Calculation of Phase Coexistence Properties and Surface Tensions of n-Alkanes with Grand-Canonical Transition-Matrix Monte Carlo Simulation and Finite-Size Scaling. Journal of Physical Chemistry B, 2006, 110, 1369-1376.	1.2	91
23	Computation of interfacial properties via grand canonical transition matrix Monte Carlo simulation. Journal of Chemical Physics, 2008, 128, 014710.	1.2	91
24	Generalized Rosenfeld scalings for tracer diffusivities in not-so-simple fluids: Mixtures and soft particles. Physical Review E, 2009, 80, 061205.	0.8	79
25	Comparative Study of the Effect of Tail Corrections on Surface Tension Determined by Molecular Simulation. Journal of Physical Chemistry B, 2007, 111, 6198-6207.	1.2	78
26	Prewetting Transitions for a Model Argon on Solid Carbon Dioxide System. Langmuir, 2004, 20, 3798-3804.	1.6	76
27	Monte Carlo Simulation Methods for Computing Liquidâ€“Vapor Saturation Properties of Model Systems. Journal of Chemical Theory and Computation, 2013, 9, 2552-2566.	2.3	76
28	Inverse design of simple pairwise interactions with low-coordinated 3D lattice ground states. Soft Matter, 2013, 9, 3866.	1.2	74
29	Solidâ€“liquid phase coexistence of the Lennard-Jones system through phase-switch Monte Carlo simulation. Journal of Chemical Physics, 2004, 120, 3130-3141.	1.2	68
30	Does confining the hard-sphere fluid between hard walls change its average properties?. Journal of Chemical Physics, 2007, 126, 244708.	1.2	65
31	Predicting How Nanoconfinement Changes the Relaxation Time of a Supercooled Liquid. Physical Review Letters, 2013, 111, 235901.	2.9	65
32	Determination of fluid-phase behavior using transition-matrix Monte Carlo: Binary Lennard-Jones mixtures. Journal of Chemical Physics, 2005, 122, 064508.	1.2	63
33	Nanoscale Limit to the Applicability of Wenzelâ€™s Equation. Langmuir, 2010, 26, 13297-13304.	1.6	61
34	On the Use of Excess Entropy Scaling to Describe the Dynamic Properties of Water. Journal of Physical Chemistry B, 2010, 114, 10558-10566.	1.2	61
35	Tuning Density Profiles and Mobility of Inhomogeneous Fluids. Physical Review Letters, 2008, 100, 106001.	2.9	60
36	Comparing the Use of Gibbs Ensemble and Grand-Canonical Transition-Matrix Monte Carlo Methods to Determine Phase Equilibria. Industrial & Engineering Chemistry Research, 2008, 47, 4533-4541.	1.8	54

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37	Communication: Generalizing Rosenfeld's excess-entropy scaling to predict long-time diffusivity in dense fluids of Brownian particles: From hard to ultrasoft interactions. Journal of Chemical Physics, 2011, 134, 081101.	1.2	51
38	A Calorimetric and Spectroscopic Study of DNA at Low Hydration. Journal of Physical Chemistry B, 2004, 108, 3098-3106.	1.2	50
39	Monte Carlo simulation methods for computing the wetting and drying properties of model systems. Journal of Chemical Physics, 2011, 135, 234102.	1.2	49
40	Wetting Behavior of Water near Nonpolar Surfaces. Journal of Physical Chemistry C, 2013, 117, 23017-23026.	1.5	48
41	Molecular Simulation of Phase Equilibria for Waterâ˜n-Butane and Waterâ˜n-Hexane Mixtures. Journal of Physical Chemistry B, 2000, 104, 4958-4963.	1.2	47
42	Monte Carlo simulation strategies for computing the wetting properties of fluids at geometrically rough surfaces. Journal of Chemical Physics, 2011, 135, 184702.	1.2	46
43	Metastability and Instability in the Lennard-Jones Fluid Investigated by Transition-Matrix Monte Carloâ€,â€¡. Journal of Physical Chemistry B, 2004, 108, 19595-19606.	1.2	45
44	Available states and available space: static properties that predict self-diffusivity of confined fluids. Journal of Statistical Mechanics: Theory and Experiment, 2009, 2009, P04006.	0.9	43
45	Determination of Henry's law constants through transition matrix Monte Carlo simulation. Fluid Phase Equilibria, 2005, 236, 58-65.	1.4	42
46	Direct evaluation of multicomponent phase equilibria using flat-histogram methods. Journal of Chemical Physics, 2005, 123, 164103.	1.2	41
47	On the Use of Excess Entropy Scaling To Describe Single-Molecule and Collective Dynamic Properties of Hydrocarbon Isomer Fluids. Journal of Physical Chemistry B, 2010, 114, 16487-16493.	1.2	40
48	Prewetting Boundary Tensions from MonteÂCarlo Simulation. Physical Review Letters, 2005, 95, 226107.	2.9	36
49	Influence of Substrate Strength on Wetting Behavior. Journal of Physical Chemistry C, 2008, 112, 12905-12913.	1.5	35
50	Coarse-Grained Strategy for Modeling Protein Stability in Concentrated Solutions. II: Phase Behavior. Biophysical Journal, 2006, 90, 1949-1960.	0.2	34
51	Impact of Small-Scale Geometric Roughness on Wetting Behavior. Langmuir, 2013, 29, 11815-11820.	1.6	34
52	Excess entropy scaling of dynamic quantities for fluids of dumbbell-shaped particles. Journal of Chemical Physics, 2010, 133, 104506.	1.2	33
53	Confinement, entropy, and single-particle dynamics of equilibrium hard-sphere mixtures. Journal of Chemical Physics, 2007, 127, 154513.	1.2	32
54	Dimensionality and Design of Isotropic Interactions that Stabilize Honeycomb, Square, Simple Cubic, and Diamond Lattices. Physical Review X, 2014, 4, .	2.8	32

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55	Composition and concentration anomalies for structure and dynamics of Gaussian-core mixtures. Journal of Chemical Physics, 2009, 131, 161101.	1.2	31
56	Mapping between long-time molecular and Brownian dynamics. Soft Matter, 2011, 7, 9859.	1.2	30
57	Impact of surface roughness on diffusion of confined fluids. Journal of Chemical Physics, 2011, 135, 154502.	1.2	30
58	Determination of surface tension in binary mixtures using transition-matrix Monte Carlo. Journal of Chemical Physics, 2006, 124, 024721.	1.2	29
59	Calculation of interfacial properties via free-energy-based molecular simulation: The influence of system size. Journal of Chemical Physics, 2010, 132, 224702.	1.2	29
60	Structure, Stability, and Rupture of Free and Supported Liquid Films and Assemblies in Molecular Simulations. Industrial & Engineering Chemistry Research, 2008, 47, 3582-3590.	1.8	28
61	Using Monte Carlo Simulation to Compute Liquidâ€“Vapor Saturation Properties of Ionic Liquids. Journal of Physical Chemistry B, 2013, 117, 8018-8030.	1.2	28
62	Molecular Simulation Study of Anisotropic Wetting. Langmuir, 2010, 26, 8274-8281.	1.6	27
63	Coarse-Grained Strategy for Modeling Protein Stability in Concentrated Solutions. III: Directional Protein Interactions. Biophysical Journal, 2007, 92, 4316-4324.	0.2	25
64	Investigation of the Phase Behavior of an Embedded Charge Protein Model through Molecular Simulation. Journal of Physical Chemistry B, 2007, 111, 12591-12598.	1.2	25
65	Saturation Properties of 1-Alkyl-3-methylimidazolium Based Ionic Liquids. Journal of Physical Chemistry B, 2014, 118, 8734-8743.	1.2	25
66	Multibody Interactions, Phase Behavior, and Clustering in Nanoparticleâ€“Polyelectrolyte Mixtures. Journal of Physical Chemistry B, 2015, 119, 14536-14550.	1.2	24
67	Using available volume to predict fluid diffusivity in random media. Physical Review E, 2006, 74, 040102.	0.8	22
68	Excess-entropy scaling of dynamics for a confined fluid of dumbbell-shaped particles. Physical Review E, 2010, 82, 041201.	0.8	22
69	Monte Carlo simulation strategies to compute interfacial and bulk properties of binary fluid mixtures. Journal of Chemical Physics, 2013, 138, 174112.	1.2	21
70	Application of the interface potential approach to calculate the wetting properties of a water model system. Molecular Simulation, 2013, 39, 1143-1152.	0.9	19
71	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
72	Implications of the effective one-component analysis of pair correlations in colloidal fluids with polydispersity. Journal of Chemical Physics, 2011, 135, 124513.	1.2	16

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73	Temperature extrapolation of multicomponent grand canonical free energy landscapes. Journal of Chemical Physics, 2017, 147, 054105.	1.2	16
74	Connection between Thermodynamics and Dynamics of Simple Fluids in Highly Attractive Pores. Langmuir, 2013, 29, 14527-14535.	1.6	15
75	Understanding the influence of Coulomb and dispersion interactions on the wetting behavior of ionic liquids. Journal of Chemical Physics, 2014, 141, 174706.	1.2	15
76	The Use of Monte Carlo Simulation to Obtain the Wetting Properties of Water. Physics Procedia, 2014, 53, 44-49.	1.2	15
77	Monte Carlo Simulation Strategies to Compute the Interfacial Properties of a Model Octaneâ€“Waterâ€“Silica System. Journal of Physical Chemistry C, 2018, 122, 17309-17318.	1.5	15
78	Fluid phase behavior of a model colloid-polymer mixture: Influence of polymer size and interaction strength. Journal of Chemical Physics, 2008, 129, 164907.	1.2	14
79	Residual multiparticle entropy does not generally change sign near freezing. Journal of Chemical Physics, 2008, 128, 161101.	1.2	14
80	Enhancing tracer diffusivity by tuning interparticle interactions and coordination shell structure. Soft Matter, 2012, 8, 4083-4089.	1.2	14
81	Understanding wetting of immiscible liquids near a solid surface using molecular simulation. Journal of Chemical Physics, 2013, 139, 064110.	1.2	14
82	Communication: Phase behavior of materials with isotropic interactions designed by inverse strategies to favor diamond and simple cubic lattice ground states. Journal of Chemical Physics, 2013, 139, 141102.	1.2	14
83	Insights Into Crowding Effects on Protein Stability From a Coarse-Grained Model. Journal of Biomechanical Engineering, 2009, 131, 071002.	0.6	13
84	Predicting low-temperature free energy landscapes with flat-histogram Monte Carlo methods. Journal of Chemical Physics, 2017, 146, 074101.	1.2	13
85	Phase Behavior of Model Confined Fluids. Influence of Substrateâ^'Fluid Interaction Strength. Journal of Physical Chemistry B, 2008, 112, 14911-14919.	1.2	12
86	Connection Between Thermodynamics and Dynamics of Simple Fluids in Pores: Impact of Fluidâ€“Fluid Interaction Range and Fluidâ€“Solid Interaction Strength. Journal of Physical Chemistry C, 2017, 121, 16316-16327.	1.5	12
87	Multivariable extrapolation of grand canonical free energy landscapes. Journal of Chemical Physics, 2017, 147, 234111.	1.2	12
88	Evaluation of the Performance of GAFF and CGenFF in the Prediction of Liquidâ€“Vapor Saturation Properties of Naphthalene Derivatives. Industrial & Engineering Chemistry Research, 2014, 53, 16072-16081.	1.8	10
89	Free energy and concentration of crystalline vacancies by molecular simulation. Molecular Physics, 2018, 116, 3027-3041.	0.8	9
90	Effect of Surface Hydrophilicity on the Interfacial Properties of a Model Octaneâ€“Waterâ€“Silica System. Journal of Physical Chemistry C, 2019, 123, 19649-19658.	1.5	9

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91	Using isothermal-isobaric Monte Carlo simulation to study the wetting behavior of model systems. Journal of Chemical Physics, 2019, 150, 084110.	1.2	9
92	Liquidâ€“Vapor Phase Behavior of Asphaltene-like Molecules. Industrial & Engineering Chemistry Research, 2014, 53, 17833-17842.	1.8	8
93	The rate of convergence of the virial series in confined systems. Molecular Physics, 2015, 113, 1179-1189.	0.8	8
94	Application of the interface potential approach for studying wetting behavior within a molecular dynamics framework. Journal of Chemical Physics, 2019, 150, 204118.	1.2	8
95	Flat-histogram extrapolation as a useful tool in the age of big data. Molecular Simulation, 2021, 47, 395-407.	0.9	7
96	Calculation of the Saturation Properties of a Model Octaneâ€“Water System Using Monte Carlo Simulation. Journal of Physical Chemistry B, 2018, 122, 6260-6271.	1.2	6
97	Coupled Monte Carlo and Molecular Dynamics Simulations on Interfacial Properties of Antifouling Polymer Membranes. Journal of Physical Chemistry B, 2021, 125, 8193-8204.	1.2	5
98	Response to â€œComment on â€˜Residual multiparticle entropy does not generally change sign near freezingâ€™â€‰â€•[J. Chem. Phys. 130, 037101 (2009)]. Journal of Chemical Physics, 2009, 130, 037102.	1.2	4
99	Position-Dependent Dynamics Explain Pore-Averaged Diffusion in Strongly Attractive Adsorptive Systems. Langmuir, 2017, 33, 13955-13963.	1.6	4
100	Construction of the interface potential from a series of canonical ensemble simulations. Journal of Chemical Physics, 2019, 151, 044103.	1.2	4
101	Improving the efficiency of Monte Carlo simulations of ions using expanded grand canonical ensembles. Journal of Chemical Physics, 2019, 151, 144109.	1.2	4
102	Effect of Carboxylic Acid on the Wetting Properties of a Model Waterâ€“Octaneâ€“Silica System. Langmuir, 2019, 35, 6540-6549.	1.6	4
103	Comments on â€œMonte Carlo simulations for water adsorption in porous materials: Best practices and new insightsâ€• AIChE Journal, 2022, 68, .	1.8	1
104	Concentration and crowding effects on protein stability from a coarse-grained model. , 2009, , 1-25.		0
105	Recent developments in the theory of amorphous aqueous systems. Special Publication - Royal Society of Chemistry, 2007, , 115-120.	0.0	0