Brian B Laird

List of Publications by Year
in descending order

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113 papers	5,784 citations	66343 42 h-index	76900 74 g-index
117 all docs	117 docs citations	117 times ranked	4210 citing authors

#	Article	IF	Citations
1	The NosÃ©â€“PoincarÃ© Method for Constant Temperature Molecular Dynamics. Journal of Computational Physics, 1999, 151, 114-134.	3.8	342
2	Atomistic characterization of the chemically heterogeneous Alâ€“Pb solidâ€“liquid interface. Acta Materialia, 2012, 60, 4960-4971.	7.9	319
3	A Combined Experimentalâ^'Computational Investigation of Carbon Dioxide Capture in a Series of Isoreticular Zeolitic Imidazolate Frameworks. Journal of the American Chemical Society, 2010, 132, 11006-11008.	13.7	303
4	Direct Calculation of the Hard-Sphere Crystal/Melt Interfacial Free Energy. Physical Review Letters, 2000, 85, 4751-4754.	7.8	245
5	Localized low-frequency vibrational modes in a simple model glass. Physical Review Letters, 1991, 66, 636-639.	7.8	240
6	Simulation of the hard-sphere crystalâ€“melt interface. Journal of Chemical Physics, 1998, 108, 9452-9462.	3.0	201
7	Localized low-frequency vibrational modes in glasses. Physical Review B, 1991, 44, 6746-6754.	3.2	187
8	Direct calculation of the crystalâ€“melt interfacial free energies for continuous potentials: Application to the Lennard-Jones system. Journal of Chemical Physics, 2003, 118, 7651.	3.0	173
9	Evaluation of the constant potential method in simulating electric double-layer capacitors. Journal of Chemical Physics, 2014, 141, 184102.	3.0	165
10	Microscopic theory of reversible pressure broadening in holeâ€burning spectra of impurities in glasses. Journal of Chemical Physics, 1989, 90, 3274-3281.	3.0	156
11	Quantumâ€mechanical derivation of the Bloch equations: Beyond the weakâ€coupling limit. Journal of Chemical Physics, 1991, 94, 4391-4404.	3.0	141
12	The anisotropic hard-sphere crystal-melt interfacial free energy from fluctuations. Journal of Chemical Physics, 2006, 125, 094710.	3.0	119
13	A Combined Experimental-Computational Study on the Effect of Topology on Carbon Dioxide Adsorption in Zeolitic Imidazolate Frameworks. Journal of Physical Chemistry C, 2012, 116, 24084-24090.	3.1	112
14	Symplectic algorithm for constant-pressure molecular dynamics using a NosÃ©â€“PoincarÃ© thermostat. Journal of Chemical Physics, 2000, 112, 3474-3482.	3.0	110
15	Crystalâ€“Melt Interfaces and Solidification Morphologies in Metals and Alloys. MRS Bulletin, 2004, 29, 935-939.	3.5	109
16	Instantaneous Normal Modes and the Glass Transition. Physical Review Letters, 1995, 74, 936-939.	7.8	107
17	Crystal Structure and Interaction Dependence of the Crystal-Melt Interfacial Free Energy. Physical Review Letters, 2005, 94, 086102.	7.8	104
18	Atomistic Simulations of Nonequilibrium Crystal-Growth Kinetics from Alloy Melts. Physical Review Letters, 2011, 107, 025505.	7.8	104

#	Article	IF	Citations
19	The crystal/liquid interface: structure and properties from computer simulation. Chemical Reviews, 1992, 92, 1819-1837.	47.7	90
20	The solidâ€“liquid interfacial free energy of close-packed metals: Hard-spheres and the Turnbull coefficient. Journal of Chemical Physics, 2001, 115, 2887-2888.	3.0	88
21	Adjusting the melting point of a model system via Gibbs-Duhem integration: Application to a model of aluminum. Physical Review B, 2000, 62, 14720-14727.	3.2	87
22	A Combined Experimentalâ€“Computational Investigation of Methane Adsorption and Selectivity in a Series of Isoreticular Zeolitic Imidazolate Frameworks. Journal of Physical Chemistry C, 2013, 117, 10326-10335.	3.1	83
23	The role of localization in glasses and supercooled liquids. Journal of Chemical Physics, 1996, 104, 5199-5208.	3.0	82
24	Phase diagram for the inverse sixth power potential system from molecular dynamics computer simulation. Molecular Physics, 1992, 75, 71-80.	1.7	79
25	Calculation of the entropy from multiparticle correlation functions. Physical Review A, 1992, 45, 5680-5689.	2.5	77
26	Density functional theory of freezing: Analysis of crystal density. Journal of Chemical Physics, 1987, 87, 5449-5456.	3.0	75
27	Freezing of soft spheres: A critical test for weighted-density-functional theories. Physical Review A, 1990, 42, 4810-4819.	2.5	75
28	Direct Calculation of the Crystalâ˜Melt Interfacial Free Energy via Molecular Dynamics Computer Simulation. Journal of Physical Chemistry B, 2005, 109, 17802-17812.	2.6	75
29	Kinetic Coefficient for Hard-Sphere Crystal Growth from the Melt. Physical Review Letters, 2006, 97, 216102.	7.8	66
30	Atomistic characterization of the Cuâ€“Pb solidâ€“liquid interface. Acta Materialia, 2011, 59, 3137-3144.	7.9	64
31	Determination of the solid-liquid interfacial free energy along a coexistence line by Gibbsâ€“Cahn integration. Journal of Chemical Physics, 2009, 131, 114110.	3.0	62
32	T2 can be greater than 2T1 even at finite temperature. Journal of Chemical Physics, 1991, 94, 4405-4410.	3.0	56
33	Phase Equilibria in Carbon Dioxide Expanded Solvents:Â Experiments and Molecular Simulations. Journal of Physical Chemistry B, 2006, 110, 13195-13202.	2.6	56
34	Solid-Liquid Interfacial Premelting. Physical Review Letters, 2013, 110, 096102.	7.8	56
35	Chemical stability of peptides in polymers. 2. Discriminating between solvent and plasticizing effects of water on peptide deamidation in poly(vinylpyrrolidone). Journal of Pharmaceutical Sciences, 1999, 88, 1081-1089.	3.3	54
36	On the connection between Gaussian statistics and excited-state linear response for time-dependent fluorescence. Journal of Chemical Physics, 2007, 126, 211104.	3.0	47

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37	Dielectric Properties of Organic Solvents in an Electric Field. Journal of Physical Chemistry C, 2017, 121, 1025-1031.	3.1	47
38	Mechanistic insights for enhancing activity and stability of Nb-incorporated silicates for selective ethylene epoxidation. Journal of Catalysis, 2016, 336, 75-84.	6.2	44
39	Freezing of the Lennard-Jones liquid. Chemical Physics Letters, 1985, 122, 320-323.	2.6	43
40	Comparison of weighted-density-functional theories for inhomogeneous liquids. Physical Review A, 1990, 42, 4806-4809.	2.5	43
41	Crystal-melt interfacial free energy of binary hard spheres from capillary fluctuations. Physical Review B, 2008, 78, .	3.2	43
42	A symplectic method for rigid-body molecular simulation. Journal of Chemical Physics, 1997, 107, 2580-2588.	3.0	42
43	On the microscopic nature of inhomogeneously broadened spectra of chromophores in glasses and crystals. Journal of Chemical Physics, 1989, 90, 3880-3881.	3.0	40
44	The crystalâ€“liquid interface of a bodyâ€centeredâ€cubicâ€forming substance: Computer simulations of the râ^'6 potential. Journal of Chemical Physics, 1989, 91, 3638-3646.	3.0	33
45	Calculation of the entropy of binary hard sphere mixtures from pair correlation functions. Journal of Chemical Physics, 1992, 97, 2153-2155.	3.0	33
46	Calculation of the crystal-melt interfacial free energy of succinonitrile from molecular simulation. Journal of Chemical Physics, 2006, 124, 044707.	3.0	33
47	Calculation of the interfacial free energy of a fluid at a static wall by Gibbsâ€“Cahn integration. Journal of Chemical Physics, 2010, 132, 204101.	3.0	31
48	Wall-Induced Prefreezing in Hard Spheres:â€‰ A Thermodynamic Perspective. Journal of Physical Chemistry C, 2007, 111, 15952-15956.	3.1	30
49	Generating generalized distributions from dynamical simulation. Journal of Chemical Physics, 2003, 118, 5759-5768.	3.0	29
50	Weighted-density approximation for general nonuniform fluid mixtures. Physical Review E, 1999, 60, 3417-3420.	2.1	28
51	Simulations of binary hard-sphere crystal-melt interfaces: Interface between a one-component fcc crystal and a binary fluid mixture. Journal of Chemical Physics, 2002, 116, 3410-3419.	3.0	28
52	Interfacial free energy of a hard-sphere fluid in contact with curved hard surfaces. Physical Review E, 2012, 86, 060602.	2.1	28
53	Simulation of the binary hard-sphere crystal/melt interface. Physical Review E, 1996, 54, R5905-R5908.	2.1	26
54	3-Hydroxy-4-nitro-cyclohexanone aus Ketonen und 4-NitrobuttersÃurechlorid. Eine ringerweiternde FÃ¼nfringanellierung. Helvetica Chimica Acta, 1981, 64, 736-760.	1.6	25

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55	Instantaneous normal modes analysis of amorphous and supercooled silica. Journal of Chemical Physics, 2001, 114, 2340-2344.	3.0	25
56	Prediction of phase equilibria and transport properties in carbon-dioxide expanded solvents by molecular simulation. Molecular Simulation, 2007, 33, 861-869.	2.0	25
57	Gas Membrane Selectivity Enabled by Zeolitic Imidazolate Framework Electrostatics. Chemistry of Materials, 2014, 26, 3976-3985.	6.7	25
58	Weightedâ€densityâ€functional theory calculation of elastic constants for faceâ€centeredâ€cubic and bodyâ€centeredâ€cubic hardâ€sphere crystals. Journal of Chemical Physics, 1992, 97, 2699-2704.	3.0	24
59	A molecular dynamics algorithm for mixed hard-core/continuous potentials. Molecular Physics, 2000, 98, 309-316.	1.7	24
60	Electric potential calculation in molecular simulation of electric double layer capacitors. Journal of Physics Condensed Matter, 2016, 28, 464006.	1.8	23
61	Octafluorocyclooctatetraene transition-metal chemistry: 1,2-.eta. and 1,2,3,6-.eta. complexes of iron and platinum. Journal of the American Chemical Society, 1981, 103, 970-972.	13.7	22
62	van der Waals density functional study of CO2binding in zeolitic imidazolate frameworks. Physical Review B, 2012, 85, .	3.2	22
63	Transport properties of CO2-expanded acetonitrile from molecular dynamics simulations. Journal of Chemical Physics, 2007, 126, 074507.	3.0	21
64	Multiple weak supramolecular interactions stabilize a surprisingly twisted As2L3 assembly. Chemical Communications, 2008, , 3936.	4.1	21
65	Time-dependent fluorescence in nanoconfined solvents: Linear-response approximations and Gaussian statistics. Journal of Chemical Physics, 2011, 135, 084511.	3.0	20
66	Molecular dynamics simulation of binary hard sphere crystal/melt interfaces. Molecular Physics, 1999, 97, 833-839.	1.7	19
67	Tunability of Gas-Expanded Liquids under Confinement: Phase Equilibrium and Transport Properties of Ethylene-Expanded Methanol in Mesoporous Silica. Journal of Physical Chemistry C, 2016, 120, 5010-5019.	3.1	17
68	Density functional theory of freezing for hexagonal symmetry: Comparison with Landau theory. Journal of Chemical Physics, 1988, 88, 3900-3909.	3.0	16
69	Inhomogeneous broadening in solids: Progress towards a microscopic understanding. Journal of Luminescence, 1990, 45, 6-8.	3.1	16
70	Origins of CH₄/CO₂ Adsorption Selectivity in Zeolitic Imidazolate Frameworks: A van der Waals Density Functional Study. Journal of Physical Chemistry C, 2013, 117, 14642-14651.	3.1	16
71	Orientation dependence of heterogeneous nucleation at the Cuâ€“Pb solid-liquid interface. Journal of Chemical Physics, 2016, 145, 211914.	3.0	16
72	A partitioned density functional theory of freezing: application to soft spheres. Molecular Physics, 1997, 90, 951-958.	1.7	15

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73	Structure and dynamics of the interface between a binary hard-sphere crystal of NaCl type and its coexisting binary fluid. Physical Review B, 2002, 66, .	3.2	12
74	Generalized dynamical thermostating technique. Physical Review E, 2003, 68, 016704.	2.1	12
75	A density functional theory study of ethylene epoxidation catalyzed by niobium-doped silica. Journal of Molecular Catalysis A, 2016, 424, 1-7.	4.8	12
76	Step-controlled Brownian motion of nanosized liquid Pb inclusions in a solid Al matrix. Acta Materialia, 2017, 141, 427-433.	7.9	12
77	Droplet spreading on a surface exhibiting solid-liquid interfacial premelting. Acta Materialia, 2018, 143, 319-328.	7.9	12
78	In-plane characterization of structural and thermodynamic properties for steps at faceted chemically heterogeneous solid/liquid interfaces. Acta Materialia, 2018, 143, 329-337.	7.9	12
79	Comment on "Entropy of hydrophobic hydration: a new statistical mechanical formulation". The Journal of Physical Chemistry, 1993, 97, 5788-5788.	2.9	11
80	Consistent integral equations for two- and three-body-force models: Application to a model of silicon. Physical Review E, 1993, 47, 2491-2502.	2.1	11
81	Amorphous Silica Slab Models with Variable Surface Roughness and Silanol Density for Use in Simulations of Dynamics and Catalysis. Journal of Physical Chemistry C, 2021, 125, 23418-23434.	3.1	11
82	Octafluorocyclooctatetraene transition-metal compounds. Novel transannular ring closures and a formal intramolecular redox equilibrium between 1,2,5,6-.eta. and 1,2,3,6-.eta. ligands. Organometallics, 1983, 2, 195-197.	2.3	10
83	Entropy of electrolytes. Journal of Chemical Physics, 1994, 100, 3775-3779.	3.0	10
84	Entropy, Disorder, and Freezing. Journal of Chemical Education, 1999, 76, 1388.	2.3	10
85	Density-Functional Methods in Chemistry: An Overview. ACS Symposium Series, 1996, , 1-17.	0.5	9
86	Monte Carlo simulations of CO2-expanded acetonitrile. Molecular Physics, 2006, 104, 2955-2960.	1.7	9
87	Thermodynamics and Intrinsic Structure of the Alâ€“Pb Liquidâ€“Liquid Interface: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2014, 118, 8373-8380.	2.6	9
88	Thermodynamics of the hard-disk fluid at a planar hard wall: Generalized scaled-particle theory and Monte Carlo simulation. Journal of Chemical Physics, 2018, 149, 084701.	3.0	9
89	Kinetics of Crystallization and Orientational Ordering in Dipolar Particle Systems. Crystal Growth and Design, 2020, 20, 7862-7873.	3.0	9
90	Localization and the glass transition. Journal of Physics Condensed Matter, 1996, 8, 9569-9573.	1.8	8

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91	Surface free energy of a hard-sphere fluid at curved walls: Deviations from morphometric thermodynamics. Journal of Chemical Physics, 2018, 149, 174706.	3.0	8
92	Hydrogen bonding in tungsten(VI) salicylate free acids1Dedicated to Professor Daryle Busch on the occasion of his 70th birthday.1. Coordination Chemistry Reviews, 1998, 174, 255-282.	18.8	7
93	On the approximation of Feynmanâ€“Kac path integrals. Journal of Computational Physics, 2003, 185, 472-483.	3.8	7
94	Pressure and Temperature Tuning of Gas-Expanded Liquid Structure and Dynamics. Journal of Physical Chemistry B, 2019, 123, 2915-2924.	2.6	7
95	Cyclopentadienylcobalt and rhodium complexes containing monocyclic and bicyclic valence isomers of octafluorocyclooctatetraene: crystal and molecular structures of the exo and endo isomers of (.eta.-cyclopentadienyl)(2-5-.eta.-octafluorobicylo[4.2.0]octa-2,4,7-triene)rhodium(I). Organometallics, 1985, 4, 1606-1611.	2.3	6
96	Molecular simulation of ethylene-expanded methanol: Phase behavior, structure, and transport properties. Fluid Phase Equilibria, 2016, 411, 81-87.	2.5	6
97	Properties of the hard-sphere fluid at a planar wall using virial series and molecular-dynamics simulation. Journal of Chemical Physics, 2018, 149, 014704.	3.0	6
98	Parameterising the surface free energy and excess adsorption of a hard-sphere fluid at a planar hard wall. Molecular Physics, 2015, 113, 1091-1096.	1.7	5
99	Structure and thermodynamics of a polar fluid at a discretely polarized wall. Molecular Physics, 2000, 98, 651-656.	1.7	4
100	A 6-site force field for succinonitrile. Molecular Physics, 2005, 103, 2795-2801.	1.7	4
101	The phase equilibrium, transport and local liquid structure of the methanol/water/ethylene ternary system: A molecular simulation study. Fluid Phase Equilibria, 2016, 429, 275-280.	2.5	4
102	On the ratio T2/T1 for nonâ€Ohmic spectral densities. Journal of Chemical Physics, 1994, 101, 852-852.	3.0	3
103	Constant-temperature molecular-dynamics algorithms for mixed hard-core/continuous potentials. Journal of Chemical Physics, 2002, 117, 1001-1009.	3.0	3
104	Phase Equilibrium, Structure, and Transport Properties of Carbon-Dioxide Expanded Liquids: A Molecular Simulation Study. ACS Symposium Series, 2009, , 41-65.	0.5	3
105	Calculation of the interfacial free energy of a binary hard-sphere fluid at a planar hard wall. Journal of Chemical Physics, 2014, 140, 024703.	3.0	3
106	Surface Free Energy of a Hard-Disk Fluid at Curved Hard Walls: Theory and Simulation. Journal of Physical Chemistry B, 2020, 124, 7938-7947.	2.6	3
107	Structure of a soft-sphere fluid at a soft repulsive wall: A comparison of weighted density-functional theories. Physical Review E, 2004, 69, 051502.	2.1	2
108	Tribute to James L. Skinner. Journal of Physical Chemistry B, 2014, 118, 7669-7670.	2.6	2

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109	Molecular Simulations of Phase Equilibria and Transport Properties in a Model CO2-Expanded Lithium Perchlorate Electrolyte. Journal of Physical Chemistry B, 2021, 125, 9341-9349.	2.6	2
110	Characterization of the Al-Ga solid-liquid interface using classical and ab initio molecular dynamics simulation. Physical Review Materials, 2020, 4, .	2.4	2
111	Phase equilibrium of a quaternary system: Methanol, ethylene, water and hydrogen peroxide. Fluid Phase Equilibria, 2018, 462, 25-30.	2.5	1
112	Inside and out: surface thermodynamics from positive to negative curvature. Journal of Chemical Physics, 0, , .	3.0	1
113	Simulation of Crystal-Melt Interfaces for a System of Binary Hard Spheres. Materials Research Society Symposia Proceedings, 2001, 701, 751.	0.1	0