Brian B Laird

List of Publications by Year
in descending order

Version: 2024-02-01

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	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
2	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
3	Kinetics of Crystallization and Orientational Ordering in Dipolar Particle Systems. Crystal Growth and Design, 2020, 20, 7862-7873.	3.0	9
4	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
5	Characterization of the Al-Ga solid-liquid interface using classical and ab initio molecular dynamics simulation. Physical Review Materials, 2020, 4, .	2.4	2
6	Pressure and Temperature Tuning of Gas-Expanded Liquid Structure and Dynamics. Journal of Physical Chemistry B, 2019, 123, 2915-2924.	2.6	7
7	Phase equilibrium of a quaternary system: Methanol, ethylene, water and hydrogen peroxide. Fluid Phase Equilibria, 2018, 462, 25-30.	2.5	1
8	Droplet spreading on a surface exhibiting solid-liquid interfacial premelting. Acta Materialia, 2018, 143, 319-328.	7.9	12
9	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
10	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
11	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
12	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
13	Dielectric Properties of Organic Solvents in an Electric Field. Journal of Physical Chemistry C, 2017, 121, 1025-1031.	3.1	47
14	Step-controlled Brownian motion of nanosized liquid Pb inclusions in a solid Al matrix. Acta Materialia, 2017, 141, 427-433.	7.9	12
15	Orientation dependence of heterogeneous nucleation at the Cuâ€“Pb solid-liquid interface. Journal of Chemical Physics, 2016, 145, 211914.	3.0	16
16	Electric potential calculation in molecular simulation of electric double layer capacitors. Journal of Physics Condensed Matter, 2016, 28, 464006.	1.8	23
17	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
18	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

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19	Molecular simulation of ethylene-expanded methanol: Phase behavior, structure, and transport properties. Fluid Phase Equilibria, 2016, 411, 81-87.	2.5	6
20	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
21	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
22	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
23	Evaluation of the constant potential method in simulating electric double-layer capacitors. Journal of Chemical Physics, 2014, 141, 184102.	3.0	165
24	Tribute to James L. Skinner. Journal of Physical Chemistry B, 2014, 118, 7669-7670.	2.6	2
25	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
26	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
27	Gas Membrane Selectivity Enabled by Zeolitic Imidazolate Framework Electrostatics. Chemistry of Materials, 2014, 26, 3976-3985.	6.7	25
28	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
29	Solid-Liquid Interfacial Premelting. Physical Review Letters, 2013, 110, 096102.	7.8	56
30	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
31	Interfacial free energy of a hard-sphere fluid in contact with curved hard surfaces. Physical Review E, 2012, 86, 060602.	2.1	28
32	Atomistic characterization of the chemically heterogeneous Alâ€“Pb solidâ€“liquid interface. Acta Materialia, 2012, 60, 4960-4971.	7.9	319
33	van der Waals density functional study of CO2binding in zeolitic imidazolate frameworks. Physical Review B, 2012, 85, .	3.2	22
34	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
35	Atomistic Simulations of Nonequilibrium Crystal-Growth Kinetics from Alloy Melts. Physical Review Letters, 2011, 107, 025505.	7.8	104
36	Atomistic characterization of the Cuâ€“Pb solidâ€“liquid interface. Acta Materialia, 2011, 59, 3137-3144.	7.9	64

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37	Time-dependent fluorescence in nanoconfined solvents: Linear-response approximations and Gaussian statistics. Journal of Chemical Physics, 2011, 135, 084511.	3.0	20
38	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
39	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
40	Phase Equilibrium, Structure, and Transport Properties of Carbon-Dioxide Expanded Liquids: A Molecular Simulation Study. ACS Symposium Series, 2009, , 41-65.	0.5	3
41	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
42	Multiple weak supramolecular interactions stabilize a surprisingly twisted As2L3 assembly. Chemical Communications, 2008, , 3936.	4.1	21
43	Crystal-melt interfacial free energy of binary hard spheres from capillary fluctuations. Physical Review B, 2008, 78, .	3.2	43
44	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
45	Prediction of phase equilibria and transport properties in carbon-dioxide expanded solvents by molecular simulation. Molecular Simulation, 2007, 33, 861-869.	2.0	25
46	Wall-Induced Prefreezing in Hard Spheres:â€‰ A Thermodynamic Perspective. Journal of Physical Chemistry C, 2007, 111, 15952-15956.	3.1	30
47	Transport properties of CO2-expanded acetonitrile from molecular dynamics simulations. Journal of Chemical Physics, 2007, 126, 074507.	3.0	21
48	Phase Equilibria in Carbon Dioxide Expanded Solvents:Â Experiments and Molecular Simulations. Journal of Physical Chemistry B, 2006, 110, 13195-13202.	2.6	56
49	Monte Carlo simulations of CO2-expanded acetonitrile. Molecular Physics, 2006, 104, 2955-2960.	1.7	9
50	Kinetic Coefficient for Hard-Sphere Crystal Growth from the Melt. Physical Review Letters, 2006, 97, 216102.	7.8	66
51	The anisotropic hard-sphere crystal-melt interfacial free energy from fluctuations. Journal of Chemical Physics, 2006, 125, 094710.	3.0	119
52	Calculation of the crystal-melt interfacial free energy of succinonitrile from molecular simulation. Journal of Chemical Physics, 2006, 124, 044707.	3.0	33
53	Crystal Structure and Interaction Dependence of the Crystal-Melt Interfacial Free Energy. Physical Review Letters, 2005, 94, 086102.	7.8	104
54	A 6-site force field for succinonitrile. Molecular Physics, 2005, 103, 2795-2801.	1.7	4

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55	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
56	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
57	Crystalâ€“Melt Interfaces and Solidification Morphologies in Metals and Alloys. MRS Bulletin, 2004, 29, 935-939.	3.5	109
58	On the approximation of Feynmanâ€“Kac path integrals. Journal of Computational Physics, 2003, 185, 472-483.	3.8	7
59	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
60	Generating generalized distributions from dynamical simulation. Journal of Chemical Physics, 2003, 118, 5759-5768.	3.0	29
61	Generalized dynamical thermostating technique. Physical Review E, 2003, 68, 016704.	2.1	12
62	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
63	Constant-temperature molecular-dynamics algorithms for mixed hard-core/continuous potentials. Journal of Chemical Physics, 2002, 117, 1001-1009.	3.0	3
64	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
65	Simulation of Crystal-Melt Interfaces for a System of Binary Hard Spheres. Materials Research Society Symposia Proceedings, 2001, 701, 751.	0.1	0
66	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
67	Instantaneous normal modes analysis of amorphous and supercooled silica. Journal of Chemical Physics, 2001, 114, 2340-2344.	3.0	25
68	Structure and thermodynamics of a polar fluid at a discretely polarized wall. Molecular Physics, 2000, 98, 651-656.	1.7	4
69	A molecular dynamics algorithm for mixed hard-core/continuous potentials. Molecular Physics, 2000, 98, 309-316.	1.7	24
70	Symplectic algorithm for constant-pressure molecular dynamics using a NosÃ©â€“PoincarÃ© thermostat. Journal of Chemical Physics, 2000, 112, 3474-3482.	3.0	110
71	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
72	Direct Calculation of the Hard-Sphere Crystal/Melt Interfacial Free Energy. Physical Review Letters, 2000, 85, 4751-4754.	7.8	245

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73	Weighted-density approximation for general nonuniform fluid mixtures. Physical Review E, 1999, 60, 3417-3420.	2.1	28
74	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
75	The NosÃ©â€“PoincarÃ© Method for Constant Temperature Molecular Dynamics. Journal of Computational Physics, 1999, 151, 114-134.	3.8	342
76	Entropy, Disorder, and Freezing. Journal of Chemical Education, 1999, 76, 1388.	2.3	10
77	Molecular dynamics simulation of binary hard sphere crystal/melt interfaces. Molecular Physics, 1999, 97, 833-839.	1.7	19
78	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
79	Simulation of the hard-sphere crystalâ€“melt interface. Journal of Chemical Physics, 1998, 108, 9452-9462.	3.0	201
80	A symplectic method for rigid-body molecular simulation. Journal of Chemical Physics, 1997, 107, 2580-2588.	3.0	42
81	A partitioned density functional theory of freezing: application to soft spheres. Molecular Physics, 1997, 90, 951-958.	1.7	15
82	Density-Functional Methods in Chemistry: An Overview. ACS Symposium Series, 1996, , 1-17.	0.5	9
83	Simulation of the binary hard-sphere crystal/melt interface. Physical Review E, 1996, 54, R5905-R5908.	2.1	26
84	The role of localization in glasses and supercooled liquids. Journal of Chemical Physics, 1996, 104, 5199-5208.	3.0	82
85	Localization and the glass transition. Journal of Physics Condensed Matter, 1996, 8, 9569-9573.	1.8	8
86	Instantaneous Normal Modes and the Glass Transition. Physical Review Letters, 1995, 74, 936-939.	7.8	107
87	On the ratio T2/T1 for nonâ€Ohmic spectral densities. Journal of Chemical Physics, 1994, 101, 852-852.	3.0	3
88	Entropy of electrolytes. Journal of Chemical Physics, 1994, 100, 3775-3779.	3.0	10
89	Comment on "Entropy of hydrophobic hydration: a new statistical mechanical formulation". The Journal of Physical Chemistry, 1993, 97, 5788-5788.	2.9	11
90	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

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91	Calculation of the entropy from multiparticle correlation functions. Physical Review A, 1992, 45, 5680-5689.	2.5	77
92	Calculation of the entropy of binary hard sphere mixtures from pair correlation functions. Journal of Chemical Physics, 1992, 97, 2153-2155.	3.0	33
93	Phase diagram for the inverse sixth power potential system from molecular dynamics computer simulation. Molecular Physics, 1992, 75, 71-80.	1.7	79
94	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
95	The crystal/liquid interface: structure and properties from computer simulation. Chemical Reviews, 1992, 92, 1819-1837.	47.7	90
96	T2 can be greater than 2T1 even at finite temperature. Journal of Chemical Physics, 1991, 94, 4405-4410.	3.0	56
97	Quantumâ€mechanical derivation of the Bloch equations: Beyond the weakâ€coupling limit. Journal of Chemical Physics, 1991, 94, 4391-4404.	3.0	141
98	Localized low-frequency vibrational modes in glasses. Physical Review B, 1991, 44, 6746-6754.	3.2	187
99	Localized low-frequency vibrational modes in a simple model glass. Physical Review Letters, 1991, 66, 636-639.	7.8	240
100	Inhomogeneous broadening in solids: Progress towards a microscopic understanding. Journal of Luminescence, 1990, 45, 6-8.	3.1	16
101	Freezing of soft spheres: A critical test for weighted-density-functional theories. Physical Review A, 1990, 42, 4810-4819.	2.5	75
102	Comparison of weighted-density-functional theories for inhomogeneous liquids. Physical Review A, 1990, 42, 4806-4809.	2.5	43
103	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
104	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
105	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
106	Density functional theory of freezing for hexagonal symmetry: Comparison with Landau theory. Journal of Chemical Physics, 1988, 88, 3900-3909.	3.0	16
107	Density functional theory of freezing: Analysis of crystal density. Journal of Chemical Physics, 1987, 87, 5449-5456.	3.0	75
108	Freezing of the Lennard-Jones liquid. Chemical Physics Letters, 1985, 122, 320-323.	2.6	43

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109	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
110	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
111	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
112	3-Hydroxy-4-nitro-cyclohexanone aus Ketonen und 4-NitrobuttersÃurechlorid. Eine ringerweiternde FÃ¼nfringanellierung. Helvetica Chimica Acta, 1981, 64, 736-760.	1.6	25
113	Inside and out: surface thermodynamics from positive to negative curvature. Journal of Chemical Physics, 0, , .	3.0	1