Allan D Mackie

List of Publications by Year
in descending order

56 papers	1,694 citations	279798 23 h-index	289244 40 g-index
58 all docs	58 docs citations	58 times ranked	1166 citing authors

#	Article	IF	Citations
1	Universal Scaling for the Exit Dynamics of Block Copolymers from Micelles at Short and Long Time Scales. Macromolecules, 2022, 55, 914-927.	4.8	4
2	Generalized Energy-Conserving Dissipative Particle Dynamics with Reactions. Journal of Chemical Theory and Computation, 2022, 18, 2503-2512.	5.3	9
3	Generalized energy-conserving dissipative particle dynamics revisited: Insight from the thermodynamics of the mesoparticle leading to an alternative heat flow model. Physical Review E, 2021, 103, 062128.	2.1	8
4	Coarse-grained mean field simulations of a triblock copolymer system. The effect of flexibility on the micellization behavior. AIP Conference Proceedings, 2019, , .	0.4	2
5	Generalised dissipative particle dynamics with energy conservation: density- and temperature-dependent potentials. Physical Chemistry Chemical Physics, 2019, 21, 24891-24911.	2.8	21
6	Coarse-grained simulations of modified Jeffamine ED900 micelles. Molecular Simulation, 2018, 44, 470-477.	2.0	1
7	Simulation Analysis of the Kinetic Exchange of Copolymer Surfactants in Micelles. Langmuir, 2017, 33, 6794-6803.	3.5	6
8	Logarithmic Exchange Kinetics in Monodisperse Copolymeric Micelles. Physical Review Letters, 2017, 118, 248001.	7.8	10
9	Physical Absorption of Green House Gases in Amines: The Influence of Functionality, Structure, and Cross-Interactions. Journal of Physical Chemistry B, 2016, 120, 13136-13143.	2.6	7
10	Chain architecture and micellization: A mean-field coarse-grained model for poly(ethylene oxide) alkyl ether surfactants. Journal of Chemical Physics, 2015, 142, 114902.	3.0	10
11	Mean-Field Coarse-Grained Model for Poly(ethylene oxide)-Poly(propylene oxide)-Poly(ethylene oxide) Triblock Copolymer Systems. Langmuir, 2015, 31, 3596-3604.	3.5	12
12	Equilibrium and Transport Properties of Primary, Secondary and Tertiary Amines by Molecular Simulation. Oil and Gas Science and Technology, 2014, 69, 833-849.	1.4	7
13	A molecular simulation study of aqueous solutions of amines and alkanolamines: mixture properties and structural analysis. Molecular Simulation, 2014, 40, 123-133.	2.0	16
14	Low Critical Micelle Concentration Discrepancy between Theory and Experiment. Journal of Physical Chemistry Letters, 2014, 5, 2027-2032.	4.6	16
15	Micellar morphological transformations for a series of linear diblock model surfactants. Journal of Chemical Physics, 2014, 140, 104905.	3.0	1
16	A Transferable Force Field for Primary, Secondary, and Tertiary Alkanolamines. Journal of Chemical Theory and Computation, 2013, 9, 2097-2103.	5.3	26
17	Transferable Force Field for Equilibrium and Transport Properties in Linear and Branched Monofunctional and Multifunctional Amines. II. Secondary and Tertiary Amines. Journal of Physical Chemistry B, 2012, 116, 6193-6202.	2.6	18
18	Model Shape Transitions of Micelles: Spheres to Cylinders and Disks. Langmuir, 2012, 28, 3730-3743.	3.5	34

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19	Transferable Force Field for Equilibrium and Transport Properties in Linear, Branched, and Bifunctional Amines I. Primary Amines. Journal of Physical Chemistry B, 2011, 115, 14617-14625.	2.6	23
20	Accurate Critical Micelle Concentrations from a Microscopic Surfactant Model. Journal of Physical Chemistry B, 2011, 115, 3434-3443.	2.6	45
21	A Transferable Force Field To Predict Phase Equilibria and Surface Tension of Ethers and Glycol Ethers. Journal of Physical Chemistry B, 2011, 115, 10654-10664.	2.6	45
22	One-pot synthesis of amino functionalized mesoporous silica materials: using simulations to understand transitions between different structures. Journal of Materials Chemistry, 2009, 19, 724-732.	6.7	19
23	Monte Carlo simulations of self-assembling hexagonal and cage-like bifunctional periodic mesoporous materials. Journal of Materials Chemistry, 2009, 19, 7848.	6.7	15
24	Anisotropic United-Atoms (AUA) Potential for Alcohols. Journal of Physical Chemistry B, 2008, 112, 9853-9863.	2.6	25
25	Near Critical Coexistence for an AUA Model of Thiophenes. Oil and Gas Science and Technology, 2008, 63, 277-282.	1.4	1
26	Effective critical point location: application to thiophenes. Molecular Simulation, 2007, 33, 777-785.	2.0	6
27	Molecular Dynamics Simulation of Acid Gas Mixtures:â€‰ A Comparison between Several Approximations. Industrial & Engineering Chemistry Research, 2007, 46, 5238-5244.	3.7	36
28	Phase Behavior of Model Surfactants in the Presence of Hybrid Particles. Journal of Physical Chemistry C, 2007, 111, 16035-16044.	3.1	21
29	Monte Carlo Simulation of Self-Assembled Ordered Hybrid Materials. Langmuir, 2007, 23, 6771-6780.	3.5	33
30	An Anisotropic United Atoms (AUA) Potential for Thiophenes. Journal of Physical Chemistry B, 2007, 111, 4460-4466.	2.6	22
31	Thermodynamic and transport properties of carbon dioxide from molecular simulation. Journal of Chemical Physics, 2007, 126, 064509.	3.0	76
32	Critical point estimation of the Lennard-Jones pure fluid and binary mixtures. Journal of Chemical Physics, 2006, 125, 054515.	3.0	83
33	Phase behavior of a model surfactantâ€“solvent system at intermediate and high densities. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2005, 270-271, 277-284.	4.7	0
34	Extension of the anisotropic united atoms intermolecular potential to amines, amides and alkanols. Fluid Phase Equilibria, 2005, 236, 25-41.	2.5	45
35	Water liquid-vapor equilibria predicted by refined ab initio derived potentials. Journal of Chemical Physics, 2005, 123, 044506.	3.0	15
36	Prediction of the critical micelle concentration in a lattice model for amphiphiles using a single-chain mean-field theory. Journal of Chemical Physics, 2005, 122, 104910.	3.0	25

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37	Optimized Intermolecular Potential for Aromatic Hydrocarbons Based on Anisotropic United Atoms. III. Polyaromatic and Naphthenoaromatic Hydrocarbons. Journal of Physical Chemistry B, 2005, 109, 2970-2976.	2.6	48
38	Transport coefficients and dynamic properties of hydrogen sulfide from molecular simulation. Journal of Chemical Physics, 2005, 123, 014505.	3.0	21
39	Optimized Intermolecular Potential for Aromatic Hydrocarbons Based on Anisotropic United Atoms. 2. Alkylbenzenes and Styrene. Journal of Physical Chemistry B, 2004, 108, 14115-14123.	2.6	37
40	Optimized Intermolecular Potential for Aromatic Hydrocarbons Based on Anisotropic United Atoms. 1. Benzene. Journal of Physical Chemistry B, 2004, 108, 14109-14114.	2.6	50
41	Comparison of the Importance Sampling Single Chain Mean Field Theory with Monte Carlo Simulation and Self-Consistent Field Calculations for Polymer Adsorption onto a Flat Wall. Macromolecules, 2004, 37, 1143-1151.	4.8	14
42	Development of an Importance Sampling Single Chain Mean Field Theory for Polymer Adsorption onto a Flat Wall. Macromolecules, 2004, 37, 1124-1133.	4.8	15
43	Sphere-to-rod transitions of micelles in model nonionic surfactant solutions. Journal of Chemical Physics, 2003, 118, 3816-3826.	3.0	40
44	The hydrophobic hydration of methane as a function of temperature from histogram reweighting Monte Carlo simulations. Journal of Chemical Physics, 2001, 114, 7527-7535.	3.0	17
45	Predicting Liquidâ€“Vapour Equilibria for Water Using anab-initioPotential from Histogram Reweighting Monte Carlo Simulations. Molecular Simulation, 2000, 24, 63-69.	2.0	4
46	Vapour-liquid coexistence curves of the united-atom and anisotropic united-atom force fields for alkane mixtures. Molecular Physics, 1999, 96, 1517-1524.	1.7	34
47	Dissipative particle dynamics with energy conservation: Modelling of heat flow. Physical Chemistry Chemical Physics, 1999, 1, 2039-2049.	2.8	59
48	Dynamic and transport properties of dissipative particle dynamics with energy conservation. Journal of Chemical Physics, 1999, 111, 5267-5276.	3.0	45
49	Dissipative particle dynamics with energy conservation. Europhysics Letters, 1997, 40, 141-146.	2.0	175
50	Aggregation Behavior of a Lattice Model for Amphiphiles. Langmuir, 1997, 13, 5022-5031.	3.5	139
51	Vapour-Liquid Phase Equilibria Predictions of Methaneâ€“Alkane Mixtures by Monte Carlo Simulation. Molecular Simulation, 1997, 19, 1-15.	2.0	79
52	Phase equilibria of a lattice model for an oilâ€“waterâ€“amphiphile mixture. Journal of Chemical Physics, 1996, 104, 3718-3725.	3.0	54
53	Monte Carlo simulations of phase equilibria for a lattice homopolymer model. Journal of Chemical Physics, 1995, 102, 1014-1023.	3.0	63
54	Constant-Pressure Monte Carlo Simulations for Lattice Models. Europhysics Letters, 1994, 27, 549-554.	2.0	21

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55	Molecular simulation of self-assembly in surfactant and protein solutions. Fluid Phase Equilibria, 1993, 82, 251-260.	2.5	13
56	Thermodynamic model of liquid-solid equilibria for natural fats and oils. Fluid Phase Equilibria, 1993, 82, 261-273.	2.5	20