Allan D Mackie

List of Publications by Citations

55 papers	1,497 citations	22 h-index	37 g-index
58 ext. papers	1,605 ext. citations	3.5 avg, IF	4.3 L-index

#	Paper	IF	Citations
55	Dissipative particle dynamics with energy conservation. *Europhysics Letters*, **1997**, 40, 141-146	1.6	152
54	Aggregation Behavior of a Lattice Model for Amphiphiles. *Langmuir*, **1997**, 13, 5022-5031	4	135
53	Vapour-Liquid Phase Equilibria Predictions of Methane–Alkane Mixtures by Monte Carlo Simulation. *Molecular Simulation*, **1997**, 19, 1-15	2	76
52	Critical point estimation of the Lennard-Jones pure fluid and binary mixtures. *Journal of Chemical Physics*, **2006**, 125, 054515	3.9	76
51	Thermodynamic and transport properties of carbon dioxide from molecular simulation. *Journal of Chemical Physics*, **2007**, 126, 064509	3.9	64
50	Monte Carlo simulations of phase equilibria for a lattice homopolymer model. *Journal of Chemical Physics*, **1995**, 102, 1014-1023	3.9	60
49	Phase equilibria of a lattice model for an oil–water–amphiphile mixture. *Journal of Chemical Physics*, **1996**, 104, 3718-3725	3.9	50
48	Optimized Intermolecular Potential for Aromatic Hydrocarbons Based on Anisotropic United Atoms. 1. Benzene. *Journal of Physical Chemistry B*, **2004**, 108, 14109-14114	3.4	48
47	Dissipative particle dynamics with energy conservation: Modelling of heat flow. *Physical Chemistry Chemical Physics*, **1999**, 1, 2039-2049	3.6	48
46	Optimized intermolecular potential for aromatic hydrocarbons based on anisotropic united atoms. III. Polyaromatic and naphthenoaromatic hydrocarbons. *Journal of Physical Chemistry B*, **2005**, 109, 2970-6	3.4	46
45	A transferable force field to predict phase equilibria and surface tension of ethers and glycol ethers. *Journal of Physical Chemistry B*, **2011**, 115, 10654-64	3.4	43
44	Extension of the anisotropic united atoms intermolecular potential to amines, amides and alkanols: Application to the problems of the 2004 Fluid Simulation Challenge. *Fluid Phase Equilibria*, **2005**, 236, 25-41	2.5	41
43	Accurate critical micelle concentrations from a microscopic surfactant model. *Journal of Physical Chemistry B*, **2011**, 115, 3434-43	3.4	38
42	Optimized Intermolecular Potential for Aromatic Hydrocarbons Based on Anisotropic United Atoms. 2. Alkylbenzenes and Styrene. *Journal of Physical Chemistry B*, **2004**, 108, 14115-14123	3.4	34
41	Molecular Dynamics Simulation of Acid Gas Mixtures: A Comparison between Several Approximations. *Industrial & Engineering Chemistry Research*, **2007**, 46, 5238-5244	3.9	33
40	Sphere-to-rod transitions of micelles in model nonionic surfactant solutions. *Journal of Chemical Physics*, **2003**, 118, 3816-3826	3.9	33
39	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	31

38	Dynamic and transport properties of dissipative particle dynamics with energy conservation. *Journal of Chemical Physics*, **1999**, 111, 5267-5276	3.9	31
37	Model shape transitions of micelles: spheres to cylinders and disks. *Langmuir*, **2012**, 28, 3730-43	4	29
36	Monte carlo simulation of self-assembled ordered hybrid materials. *Langmuir*, **2007**, 23, 6771-80	4	29
35	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	3.9	24
34	Anisotropic united-atoms (AUA) potential for alcohols. *Journal of Physical Chemistry B*, **2008**, 112, 9853-63	3.4	23
33	A Transferable Force Field for Primary, Secondary, and Tertiary Alkanolamines. *Journal of Chemical Theory and Computation*, **2013**, 9, 2097-103	6.4	22
32	Transferable force field for equilibrium and transport properties in linear, branched, and bifunctional amines I. Primary amines. *Journal of Physical Chemistry B*, **2011**, 115, 14617-25	3.4	22
31	An anisotropic united atoms (AUA) potential for thiophenes. *Journal of Physical Chemistry B*, **2007**, 111, 4460-6	3.4	21
30	Constant-Pressure Monte Carlo Simulations for Lattice Models. *Europhysics Letters*, **1994**, 27, 549-554	1.6	20
29	Thermodynamic model of liquid-solid equilibria for natural fats and oils. *Fluid Phase Equilibria*, **1993**, 82, 261-273	2.5	20
28	Transport coefficients and dynamic properties of hydrogen sulfide from molecular simulation. *Journal of Chemical Physics*, **2005**, 123, 014505	3.9	19
27	Phase Behavior of Model Surfactants in the Presence of Hybrid Particles *Journal of Physical Chemistry C*, **2007**, 111, 16035-16044	3.8	17
26	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, 6193-202	3.4	16
25	The hydrophobic hydration of methane as a function of temperature from histogram reweighting Monte Carlo simulations. *Journal of Chemical Physics*, **2001**, 114, 7527-7535	3.9	16
24	Low Critical Micelle Concentration Discrepancy between Theory and Experiment. *Journal of Physical Chemistry Letters*, **2014**, 5, 2027-32	6.4	15
23	A molecular simulation study of aqueous solutions of amines and alkanolamines: mixture properties and structural analysis. *Molecular Simulation*, **2014**, 40, 123-133	2	15
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		15
21	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	5.5	14

20	Development of an Importance Sampling Single Chain Mean Field Theory for Polymer Adsorption onto a Flat Wall. *Macromolecules*, **2004**, 37, 1124-1133	5.5	14
19	Water liquid-vapor equilibria predicted by refined ab initio derived potentials. *Journal of Chemical Physics*, **2005**, 123, 044506	3.9	14
18	Molecular simulation of self-assembly in surfactant and protein solutions. *Fluid Phase Equilibria*, **1993**, 82, 251-260	2.5	13
17	Mean-field coarse-grained model for poly(ethylene oxide)-poly(propylene oxide)-poly(ethylene oxide) triblock copolymer systems. *Langmuir*, **2015**, 31, 3596-604	4	12
16	Monte Carlo simulations of self-assembling hexagonal and cage-like bifunctional periodic mesoporous materials. *Journal of Materials Chemistry*, **2009**, 19, 7848		10
15	Generalised dissipative particle dynamics with energy conservation: density- and temperature-dependent potentials. *Physical Chemistry Chemical Physics*, **2019**, 21, 24891-24911	3.6	10
14	Logarithmic Exchange Kinetics in Monodisperse Copolymeric Micelles. *Physical Review Letters*, **2017** , 118, 248001	7.4	7
13	Equilibrium and Transport Properties of Primary, Secondary and Tertiary Amines by Molecular Simulation. *Oil and Gas Science and Technology*, **2014**, 69, 833-849	1.9	6
12	Effective critical point location: application to thiophenes. *Molecular Simulation*, **2007**, 33, 777-785	2	6
11	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	3.4	6
10	Simulation Analysis of the Kinetic Exchange of Copolymer Surfactants in Micelles. *Langmuir*, **2017**, 33, 6794-6803	4	5
9	Chain architecture and micellization: a mean-field coarse-grained model for poly(ethylene oxide) alkyl ether surfactants. *Journal of Chemical Physics*, **2015**, 142, 114902	3.9	5
8	Predicting Liquid–Vapour Equilibria for Water Using an ab-initio Potential from Histogram Reweighting Monte Carlo Simulations. *Molecular Simulation*, **2000**, 24, 63-69	2	4
7	Coarse-grained mean field simulations of a triblock copolymer system. The effect of flexibility on the micellization behavior **2019**,		2
6	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	2.4	2
5	Micellar morphological transformations for a series of linear diblock model surfactants. *Journal of Chemical Physics*, **2014**, 140, 104905	3.9	1
4	Near Critical Coexistence for an AUA Model of Thiophenes. *Oil and Gas Science and Technology*, **2008**, 63, 277-282	1.9	1
3	Coarse-grained simulations of modified Jeffamine ED900 micelles. *Molecular Simulation*, **2018**, 44, 470-477		0

2	Universal Scaling for the Exit Dynamics of Block Copolymers from Micelles at Short and Long Time Scales.. *Macromolecules*, **2022**, 55, 914-927	5.5	0
1	Phase behavior of a model surfactant–solvent system at intermediate and high densities. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2005**, 270-271, 277-284	5.1	