Ruth Lynden-Bell

List of Publications by Year
in descending order

83	5,185	87888 38	82547 72
papers	citations	h-index	g-index

85	85	85	3815
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Intermolecular potentials for simulations of liquid imidazolium salts. Molecular Physics, 2001, 99, 801-809.	1.7	378
2	A Simulation Study of Waterâ"Dialkylimidazolium Ionic Liquid Mixtures. Journal of Physical Chemistry B, 2003, 107, 10873-10878.	2.6	378
3	Solvation of small molecules in imidazolium ionic liquids: a simulation study. Green Chemistry, 2002, 4, 107-111.	9.0	271
4	Ab Initio Molecular Dynamics Simulation of a Room Temperature Ionic Liquid. Journal of Physical Chemistry B, 2005, 109, 5895-5902.	2.6	269
5	Simulations of Ionic Liquids, Solutions, and Surfaces. Accounts of Chemical Research, 2007, 40, 1138-1145.	15.6	267
6	From hydrophobic to hydrophilic behaviour: A simulation study of solvation entropy and free energy of simple solutes. Journal of Chemical Physics, 1997, 107, 1981-1991.	3.0	235
7	Ab initio simulation of charged slabs at constant chemical potential. Journal of Chemical Physics, 2001, 115, 1661-1669.	3.0	206
8	Structure and Dynamics of a Confined Ionic Liquid. Topics of Relevance to Dye-Sensitized Solar Cells. Journal of Physical Chemistry B, 2005, 109, 17922-17927.	2.6	202
9	Simulation of the surface structure of butylmethylimidazolium ionic liquids. Physical Chemistry Chemical Physics, 2006, 8, 949-954.	2.8	168
10	Gasâ€"liquid interfaces of room temperature ionic liquids. Molecular Physics, 2003, 101, 2625-2633.	1.7	156
11	A model for strongly hindered molecular reorientation in liquids. The Journal of Physical Chemistry, 1984, 88, 6514-6518.	2.9	138
12	Polarization Relaxation in an Ionic Liquid Confined between Electrified Wallsâ€. Journal of Physical Chemistry B, 2007, 111, 4877-4884.	2.6	138
13	A computational investigation of thermodynamics, structure, dynamics and solvation behavior in modified water models. Journal of Chemical Physics, 2008, 128, 124511.	3.0	134
14	Chemical potentials of water and organic solutes in imidazolium ionic liquids: a simulation study. Molecular Physics, 2002, 100, 3225-3229.	1.7	125
15	Electrode screening by ionic liquids. Physical Chemistry Chemical Physics, 2012, 14, 2693.	2.8	122
16	Simulation of interfaces between room temperature ionic liquids and other liquids. Faraday Discussions, 2005, 129, 57.	3.2	118
17	Probing the neutral grapheneâ€"ionic liquid interface: insights from molecular dynamics simulations. Physical Chemistry Chemical Physics, 2012, 14, 2552.	2.8	112
18	Macroscopic and microscopic properties of solutions of aromatic compounds in an ionic liquid. Molecular Physics, 2004, 102, 85-94.	1.7	110

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19	Is a Stern and diffuse layer model appropriate to ionic liquids at surfaces?. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, E4121.	7.1	93
20	The electrostatic properties of water molecules in condensed phases: anab initiostudy. Molecular Physics, 1999, 96, 1683-1693.	1.7	92
21	Computational Investigation of Order, Structure, and Dynamics in Modified Water Modelsâ€. Journal of Physical Chemistry B, 2005, 109, 6527-6534.	2.6	88
22	Can Marcus Theory Be Applied to Redox Processes in Ionic Liquids? A Comparative Simulation Study of Dimethylimidazolium Liquids and Acetonitrile. Journal of Physical Chemistry B, 2007, 111, 10800-10806.	2.6	75
23	The structure and spectroscopy of monolayers of water on MgO: An ab initio study. Journal of Chemical Physics, 2000, 113, 3344-3350.	3.0	67
24	The surface structure of ionic liquids: Comparing simulations with x-ray measurements. Journal of Chemical Physics, 2006, 125, 174715.	3.0	67
25	Screening of pairs of ions dissolved in ionic liquids. Physical Chemistry Chemical Physics, 2010, 12, 1733-1740.	2.8	67
26	A molecular dynamics study of the structure of water layers adsorbed on MgO(100). Journal of Chemical Physics, 1998, 109, 3245-3254.	3.0	59
27	Molecular dynamics simulations of the structure of the grapheneâ€“ionic liquid/alkali salt mixtures interface. Physical Chemistry Chemical Physics, 2014, 16, 13271-13278.	2.8	58
28	Screening of Ionâ€“Graphene Electrode Interactions by Ionic Liquids: The Effects of Liquid Structure. Journal of Physical Chemistry C, 2014, 118, 5841-5847.	3.1	54
29	Does solvation cause symmetry breaking in the I3â^' ion in aqueous solution?. Journal of Chemical Physics, 1998, 109, 9928-9937.	3.0	52
30	Clusters, Liquids, and Crystals of Dialkyimidazolium Salts. A Combined Perspective from ab Initio and Classical Computer Simulations. Accounts of Chemical Research, 2007, 40, 1156-1164.	15.6	47
31	Solvation in modified water models: towards understanding hydrophobic effects. Molecular Physics, 2006, 104, 3593-3605.	1.7	45
32	Molecular dynamics simulation of the behaviour of water in nano-confined ionic liquidâ€“water mixtures. Journal of Physics Condensed Matter, 2016, 28, 464001.	1.8	44
33	Molecular electrostatic properties of ions in an ionic liquid. Molecular Physics, 2006, 104, 2477-2483.	1.7	43
34	Using simulation to study solvation in water. Pure and Applied Chemistry, 2001, 73, 1721-1731.	1.9	41
35	A molecular dynamics study of orientational disordering in crystalline sodium nitrate. Journal of Physics Condensed Matter, 1989, 1, 6523-6542.	1.8	40
36	Molecular origin of high free energy barriers for alkali metal ion transfer through ionic liquidâ€“graphene electrode interfaces. Physical Chemistry Chemical Physics, 2016, 18, 1302-1310.	2.8	39

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37	The surface-ordered phase of liquid heptadecane: a simulation study. Molecular Physics, 1999, 96, 249-257.	1.7	38
38	Density Functional Theory Study of Tetrathiafulvalene and Thianthrene in Acetonitrile:Â Structure, Dynamics, and Redox Propertiesâ€. Journal of Physical Chemistry B, 2006, 110, 3614-3623.	2.6	38
39	Is the hydrophobic effect unique to water? The relation between solvation properties and network structure in water and modified water models. Molecular Physics, 2001, 99, 1011-1021.	1.7	34
40	Local structure and intermolecular dynamics of an equimolar benzene and 1,3-dimethylimidazolium bis[(trifluoromethane)sulfonyl]amide mixture: Molecular dynamics simulations and OKE spectroscopic measurements. Journal of Chemical Physics, 2014, 141, 044506.	3.0	30
41	The behaviour of liquid alkanes near interfaces. Molecular Physics, 2000, 98, 255-260.	1.7	29
42	Phase diagrams and surface properties of modified water models. Molecular Physics, 2007, 105, 3029-3033.	1.7	29
43	Hydrogen bond strength and network structure effects on hydration of non-polar molecules. Physical Chemistry Chemical Physics, 2011, 13, 2748-2757.	2.8	28
44	Simulations of imidazolium ionic liquids: when does the cation charge distribution matter?. Journal of Physics Condensed Matter, 2009, 21, 424120.	1.8	26
45	An OHD-RIKES and simulation study comparing a benzylmethylimidazolium ionic liquid with an equimolar mixture of dimethylimidazolium and benzene. Physical Chemistry Chemical Physics, 2015, 17, 9973-9983.	2.8	26
46	Redox potentials and screening in ionic liquids: Effects of sizes and shapes of solute ions. Journal of Chemical Physics, 2008, 129, 204503.	3.0	21
47	Surfactant structure around DNA in aqueous solution. Physical Chemistry Chemical Physics, 2000, 2, 1305-1310.	2.8	20
48	Landau free energy curves for melting of quantum solids. Journal of Chemical Physics, 2000, 113, 9239-9247.	3.0	18
49	Molecular dynamics simulations of the structure and single-particle dynamics of mixtures of divalent salts and ionic liquids. Journal of Chemical Physics, 2015, 143, 124507.	3.0	17
50	Interactions of triiodide cluster ion with solvents. European Physical Journal D, 2005, 34, 129-132.	1.3	16
51	Nonlinear Relaxation in Redox Processes in Ionic and Polar Liquids. Journal of Physical Chemistry C, 2008, 112, 14538-14544.	3.1	16
52	Temperature and solvent dependence of vibrational relaxation of tri-iodide: A simulation study. Journal of Chemical Physics, 2003, 119, 6119-6131.	3.0	15
53	Solvent-induced symmetry breaking: Varying solvent strength. Physical Review E, 2005, 71, 021502.	2.1	14
54	Determining surface free energies of crystals with highly disordered surfaces from simulation. Molecular Physics, 1999, 96, 1027-1032.	1.7	12

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55	Using DL_POLY to study the sensitivity of liquid structure to potential parameters. Molecular Simulation, 2006, 32, 1025-1033.	2.0	12
56	Estimation of slow diffusion rates in confined systems: CCl4in zeolite NaA. Molecular Physics, 2002, 100, 641-647.	1.7	11
57	Optical Kerr effect spectroscopy of CS₂ in monocationic and dicationic ionic liquids: insights into the intermolecular interactions in ionic liquids. Physical Chemistry Chemical Physics, 2018, 20, 26558-26569.	2.8	11
58	Transfer of a pollutant molecule through a water film on a single crystal surface. Journal of Chemical Physics, 1999, 111, 4862-4864.	3.0	9
59	Solvation effects on equilibria: Triazoles and N-methyl piperidinol. Physical Chemistry Chemical Physics, 2002, 4, 5281-5288.	2.8	9
60	Towards understanding water: simulation of modified water models. Journal of Physics Condensed Matter, 2010, 22, 284107.	1.8	9
61	Exact quantum solutions of extraordinary N -body problems. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 1999, 455, 3261-3284.	2.1	8
62	A simulation study of vibrational relaxation of Iâˆ’3in liquids. Molecular Physics, 2003, 101, 1641-1649.	1.7	8
63	Hydrophobic solvation of Gayâ€“Berne particles in modified water models. Journal of Chemical Physics, 2008, 128, 104506.	3.0	8
64	The importance of polarizability: comparison of models of carbon disulphide in the ionic liquids [C1C1im][NTf2] and [C4C1im][NTf2]. Physical Chemistry Chemical Physics, 2016, 18, 16535-16543.	2.8	8
65	A simulation study of CS2 solutions in two related ionic liquids with dications and monocations. Journal of Chemical Physics, 2018, 148, 193844.	3.0	8
66	Structure and dynamics of ionic liquids: general discussion. Faraday Discussions, 2018, 206, 291-337.	3.2	8
67	The surface-ordered phase of liquid heptadecane: a simulation study. Molecular Physics, 1999, 96, 249-257.	1.7	7
68	The velocity distribution of desorbing molecules: a simulation study. Molecular Physics, 1999, 97, 1029-1034.	1.7	6
69	A simulation study of films of n-hexane and n-perfluorohexane on a solid surface. Molecular Physics, 2001, 99, 1407-1411.	1.7	6
70	Determining the electronic structure and chemical potentials of molecules in solution. Physical Chemistry Chemical Physics, 2002, 4, 3016-3021.	2.8	6
71	A model with charges and polarizability for CS2 in an ionic liquid. Journal of Chemical Sciences, 2017, 129, 883-890.	1.5	6
72	On the shapes of Newton's revolving orbits. Notes and Records of the Royal Society, 1997, 51, 195-198.	0.3	4

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73	Computed vibrational wavenumbers in ammonium fluoride crystals. Journal of Raman Spectroscopy, 2001, 32, 996-999.	2.5	3
74	Predicting cavity formation free energy: how far is the Gaussian approximation valid?. Physical Chemistry Chemical Physics, 2012, 14, 6996.	2.8	2
75	Long range corrections for charged systems. , 1999, , .		1
76	Comparison of three related imidazolium ionic liquids and their CS₂ solutions. Molecular Physics, 2020, 118, e1580782.	1.7	1
77	Determining surface free energies of crystals with highly disordered surfaces from simulation. Molecular Physics, 1999, 96, 1027-1032.	1.7	1
78	Molecular Structure and Dynamics. , 0, , 127-173.		0
79	Properties of Liquids Made from Modified Water Models. , 2010, , 89-99.		0
80	Lennardâ€"Jones Lecture 2017*. Molecular Physics, 2018, 116, 1915-1920.	1.7	0
81	Ionic liquids at interfaces: general discussion. Faraday Discussions, 2018, 206, 549-586.	3.2	0
82	Screening of highly charged ions in an ionic liquid; when will ion pairs form?. Physical Chemistry Chemical Physics, 2020, 22, 10911-10916.	2.8	0
83	My Life in Changing Times: New Ideas and New Techniques. Annual Review of Physical Chemistry, 2021, 72, 35-50.	10.8	0