

Ruth Lynden-Bell

List of Publications by Year in descending order

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83
papers

5,185
citations

87888

38
h-index

82547

72
g-index

85
all docs

85
docs citations

85
times ranked

3815
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|--|------|-----------|
| 1 | My Life in Changing Times: New Ideas and New Techniques. Annual Review of Physical Chemistry, 2021, 72, 35-50. | 10.8 | 0 |
| 2 | Comparison of three related imidazolium ionic liquids and their CS ₂ solutions. Molecular Physics, 2020, 118, e1580782. | 1.7 | 1 |
| 3 | 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 |
| 4 | Lennard-Jones Lecture 2017*. Molecular Physics, 2018, 116, 1915-1920. | 1.7 | 0 |
| 5 | A simulation study of CS ₂ solutions in two related ionic liquids with dications and monocations. Journal of Chemical Physics, 2018, 148, 193844. | 3.0 | 8 |
| 6 | Structure and dynamics of ionic liquids: general discussion. Faraday Discussions, 2018, 206, 291-337. | 3.2 | 8 |
| 7 | Ionic liquids at interfaces: general discussion. Faraday Discussions, 2018, 206, 549-586. | 3.2 | 0 |
| 8 | Optical Kerr effect spectroscopy of CS ₂ 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 |
| 9 | A model with charges and polarizability for CS ₂ in an ionic liquid. Journal of Chemical Sciences, 2017, 129, 883-890. | 1.5 | 6 |
| 10 | 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 |
| 11 | Molecular dynamics simulation of the behaviour of water in nano-confined ionic liquid-water mixtures. Journal of Physics Condensed Matter, 2016, 28, 464001. | 1.8 | 44 |
| 12 | Molecular origin of high free energy barriers for alkali metal ion transfer through ionic liquid-graphene electrode interfaces. Physical Chemistry Chemical Physics, 2016, 18, 1302-1310. | 2.8 | 39 |
| 13 | 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 |
| 14 | 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 |
| 15 | 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 |
| 16 | Molecular dynamics simulations of the structure of the graphene-ionic liquid/alkali salt mixtures interface. Physical Chemistry Chemical Physics, 2014, 16, 13271-13278. | 2.8 | 58 |
| 17 | Screening of Ion-Graphene Electrode Interactions by Ionic Liquids: The Effects of Liquid Structure. Journal of Physical Chemistry C, 2014, 118, 5841-5847. | 3.1 | 54 |
| 18 | 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 |

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|----|--|------|-----------|
| 19 | Probing the neutral graphene-ionic liquid interface: insights from molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 2552. | 2.8 | 112 |
| 20 | Predicting cavity formation free energy: how far is the Gaussian approximation valid?. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 6996. | 2.8 | 2 |
| 21 | Electrode screening by ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 2693. | 2.8 | 122 |
| 22 | Hydrogen bond strength and network structure effects on hydration of non-polar molecules. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2748-2757. | 2.8 | 28 |
| 23 | Properties of Liquids Made from Modified Water Models. , 2010, , 89-99. | | 0 |
| 24 | Screening of pairs of ions dissolved in ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1733-1740. | 2.8 | 67 |
| 25 | Towards understanding water: simulation of modified water models. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 284107. | 1.8 | 9 |
| 26 | Simulations of imidazolium ionic liquids: when does the cation charge distribution matter?. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 424120. | 1.8 | 26 |
| 27 | Nonlinear Relaxation in Redox Processes in Ionic and Polar Liquids. <i>Journal of Physical Chemistry C</i> , 2008, 112, 14538-14544. | 3.1 | 16 |
| 28 | Redox potentials and screening in ionic liquids: Effects of sizes and shapes of solute ions. <i>Journal of Chemical Physics</i> , 2008, 129, 204503. | 3.0 | 21 |
| 29 | Hydrophobic solvation of Gay-Berne particles in modified water models. <i>Journal of Chemical Physics</i> , 2008, 128, 104506. | 3.0 | 8 |
| 30 | A computational investigation of thermodynamics, structure, dynamics and solvation behavior in modified water models. <i>Journal of Chemical Physics</i> , 2008, 128, 124511. | 3.0 | 134 |
| 31 | Phase diagrams and surface properties of modified water models. <i>Molecular Physics</i> , 2007, 105, 3029-3033. | 1.7 | 29 |
| 32 | Can Marcus Theory Be Applied to Redox Processes in Ionic Liquids? A Comparative Simulation Study of Dimethylimidazolium Liquids and Acetonitrile. <i>Journal of Physical Chemistry B</i> , 2007, 111, 10800-10806. | 2.6 | 75 |
| 33 | Clusters, Liquids, and Crystals of Dialkylimidazolium Salts. A Combined Perspective from ab Initio and Classical Computer Simulations. <i>Accounts of Chemical Research</i> , 2007, 40, 1156-1164. | 15.6 | 47 |
| 34 | Simulations of Ionic Liquids, Solutions, and Surfaces. <i>Accounts of Chemical Research</i> , 2007, 40, 1138-1145. | 15.6 | 267 |
| 35 | Polarization Relaxation in an Ionic Liquid Confined between Electrified Walls. <i>Journal of Physical Chemistry B</i> , 2007, 111, 4877-4884. | 2.6 | 138 |
| 36 | Density Functional Theory Study of Tetrathiafulvalene and Thianthrene in Acetonitrile: Structure, Dynamics, and Redox Properties. <i>Journal of Physical Chemistry B</i> , 2006, 110, 3614-3623. | 2.6 | 38 |

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|----|--|-----|-----------|
| 37 | Simulation of the surface structure of butylmethylimidazolium ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 949-954. | 2.8 | 168 |
| 38 | The surface structure of ionic liquids: Comparing simulations with x-ray measurements. <i>Journal of Chemical Physics</i> , 2006, 125, 174715. | 3.0 | 67 |
| 39 | Solvation in modified water models: towards understanding hydrophobic effects. <i>Molecular Physics</i> , 2006, 104, 3593-3605. | 1.7 | 45 |
| 40 | Using DL_POLY to study the sensitivity of liquid structure to potential parameters. <i>Molecular Simulation</i> , 2006, 32, 1025-1033. | 2.0 | 12 |
| 41 | Molecular electrostatic properties of ions in an ionic liquid. <i>Molecular Physics</i> , 2006, 104, 2477-2483. | 1.7 | 43 |
| 42 | Interactions of triiodide cluster ion with solvents. <i>European Physical Journal D</i> , 2005, 34, 129-132. | 1.3 | 16 |
| 43 | Solvent-induced symmetry breaking: Varying solvent strength. <i>Physical Review E</i> , 2005, 71, 021502. | 2.1 | 14 |
| 44 | Simulation of interfaces between room temperature ionic liquids and other liquids. <i>Faraday Discussions</i> , 2005, 129, 57. | 3.2 | 118 |
| 45 | Ab Initio Molecular Dynamics Simulation of a Room Temperature Ionic Liquid. <i>Journal of Physical Chemistry B</i> , 2005, 109, 5895-5902. | 2.6 | 269 |
| 46 | Computational Investigation of Order, Structure, and Dynamics in Modified Water Models. <i>Journal of Physical Chemistry B</i> , 2005, 109, 6527-6534. | 2.6 | 88 |
| 47 | Structure and Dynamics of a Confined Ionic Liquid. <i>Topics of Relevance to Dye-Sensitized Solar Cells. Journal of Physical Chemistry B</i> , 2005, 109, 17922-17927. | 2.6 | 202 |
| 48 | Macroscopic and microscopic properties of solutions of aromatic compounds in an ionic liquid. <i>Molecular Physics</i> , 2004, 102, 85-94. | 1.7 | 110 |
| 49 | A Simulation Study of Water in Dialkylimidazolium Ionic Liquid Mixtures. <i>Journal of Physical Chemistry B</i> , 2003, 107, 10873-10878. | 2.6 | 378 |
| 50 | Gas-liquid interfaces of room temperature ionic liquids. <i>Molecular Physics</i> , 2003, 101, 2625-2633. | 1.7 | 156 |
| 51 | A simulation study of vibrational relaxation of I ₃ in liquids. <i>Molecular Physics</i> , 2003, 101, 1641-1649. | 1.7 | 8 |
| 52 | Temperature and solvent dependence of vibrational relaxation of tri-iodide: A simulation study. <i>Journal of Chemical Physics</i> , 2003, 119, 6119-6131. | 3.0 | 15 |
| 53 | Solvation of small molecules in imidazolium ionic liquids: a simulation study. <i>Green Chemistry</i> , 2002, 4, 107-111. | 9.0 | 271 |
| 54 | Solvation effects on equilibria: Triazoles and N-methyl piperidinol. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5281-5288. | 2.8 | 9 |

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| 55 | Determining the electronic structure and chemical potentials of molecules in solution. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 3016-3021. | 2.8 | 6 |
| 56 | Estimation of slow diffusion rates in confined systems: CCl ₄ in zeolite NaA. <i>Molecular Physics</i> , 2002, 100, 641-647. | 1.7 | 11 |
| 57 | Chemical potentials of water and organic solutes in imidazolium ionic liquids: a simulation study. <i>Molecular Physics</i> , 2002, 100, 3225-3229. | 1.7 | 125 |
| 58 | Intermolecular potentials for simulations of liquid imidazolium salts. <i>Molecular Physics</i> , 2001, 99, 801-809. | 1.7 | 378 |
| 59 | A simulation study of films of n-hexane and n-perfluorohexane on a solid surface. <i>Molecular Physics</i> , 2001, 99, 1407-1411. | 1.7 | 6 |
| 60 | Using simulation to study solvation in water. <i>Pure and Applied Chemistry</i> , 2001, 73, 1721-1731. | 1.9 | 41 |
| 61 | Computed vibrational wavenumbers in ammonium fluoride crystals. <i>Journal of Raman Spectroscopy</i> , 2001, 32, 996-999. | 2.5 | 3 |
| 62 | Is the hydrophobic effect unique to water? The relation between solvation properties and network structure in water and modified water models. <i>Molecular Physics</i> , 2001, 99, 1011-1021. | 1.7 | 34 |
| 63 | Ab initio simulation of charged slabs at constant chemical potential. <i>Journal of Chemical Physics</i> , 2001, 115, 1661-1669. | 3.0 | 206 |
| 64 | The behaviour of liquid alkanes near interfaces. <i>Molecular Physics</i> , 2000, 98, 255-260. | 1.7 | 29 |
| 65 | The structure and spectroscopy of monolayers of water on MgO: An ab initio study. <i>Journal of Chemical Physics</i> , 2000, 113, 3344-3350. | 3.0 | 67 |
| 66 | Landau free energy curves for melting of quantum solids. <i>Journal of Chemical Physics</i> , 2000, 113, 9239-9247. | 3.0 | 18 |
| 67 | Surfactant structure around DNA in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 1305-1310. | 2.8 | 20 |
| 68 | Determining surface free energies of crystals with highly disordered surfaces from simulation. <i>Molecular Physics</i> , 1999, 96, 1027-1032. | 1.7 | 12 |
| 69 | The velocity distribution of desorbing molecules: a simulation study. <i>Molecular Physics</i> , 1999, 97, 1029-1034. | 1.7 | 6 |
| 70 | The electrostatic properties of water molecules in condensed phases: an ab initio study. <i>Molecular Physics</i> , 1999, 96, 1683-1693. | 1.7 | 92 |
| 71 | Transfer of a pollutant molecule through a water film on a single crystal surface. <i>Journal of Chemical Physics</i> , 1999, 111, 4862-4864. | 3.0 | 9 |
| 72 | Exact quantum solutions of extraordinary N-body problems. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 1999, 455, 3261-3284. | 2.1 | 8 |

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|----|--|-----|-----------|
| 73 | The surface-ordered phase of liquid heptadecane: a simulation study. <i>Molecular Physics</i> , 1999, 96, 249-257. | 1.7 | 38 |
| 74 | Long range corrections for charged systems. , 1999, , . | | 1 |
| 75 | Determining surface free energies of crystals with highly disordered surfaces from simulation. <i>Molecular Physics</i> , 1999, 96, 1027-1032. | 1.7 | 1 |
| 76 | The surface-ordered phase of liquid heptadecane: a simulation study. <i>Molecular Physics</i> , 1999, 96, 249-257. | 1.7 | 7 |
| 77 | Does solvation cause symmetry breaking in the I3^{a} ion in aqueous solution?. <i>Journal of Chemical Physics</i> , 1998, 109, 9928-9937. | 3.0 | 52 |
| 78 | A molecular dynamics study of the structure of water layers adsorbed on MgO(100). <i>Journal of Chemical Physics</i> , 1998, 109, 3245-3254. | 3.0 | 59 |
| 79 | On the shapes of Newton's revolving orbits. <i>Notes and Records of the Royal Society</i> , 1997, 51, 195-198. | 0.3 | 4 |
| 80 | From hydrophobic to hydrophilic behaviour: A simulation study of solvation entropy and free energy of simple solutes. <i>Journal of Chemical Physics</i> , 1997, 107, 1981-1991. | 3.0 | 235 |
| 81 | A molecular dynamics study of orientational disordering in crystalline sodium nitrate. <i>Journal of Physics Condensed Matter</i> , 1989, 1, 6523-6542. | 1.8 | 40 |
| 82 | A model for strongly hindered molecular reorientation in liquids. <i>The Journal of Physical Chemistry</i> , 1984, 88, 6514-6518. | 2.9 | 138 |
| 83 | <i>Molecular Structure and Dynamics</i> . , 0, , 127-173. | | 0 |