Barbara Kirchner

List of Publications by Year
in descending order

184	11,730	22099	30848
papers	citations	59 h-index	102 g-index

192	192	192	8033
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Recognition in Chiral Ionic Liquids: The Achiral Cation Makes the Difference!. Journal of Organic Chemistry, 2022, 87, 1867-1873.	1.7	6
2	Hydrogen Bonding and Vaporization Thermodynamics in Hexafluoroisopropanolâ€Acetone and â€Methanol Mixtures. A Joined Cluster Analysis and Molecular Dynamic Study. ChemPhysChem, 2022, 23, .	1.0	9
3	Benchmarking the Computational Costs and Quality of Vibrational Spectra from Ab Initio Simulations. Advanced Theory and Simulations, 2022, 5, 2100293.	1.3	8
4	Charge transfer and polarisability in ionic liquids: a case study. Physical Chemistry Chemical Physics, 2022, 24, 3144-3162.	1.3	11
5	Chemistry Dissolved in Ionic Liquids. A Theoretical Perspective. Journal of Physical Chemistry B, 2022, 126, 766-777.	1.2	9
6	Ionic Liquid-Based Low-Temperature Synthesis of Crystalline Ti(OH)OFÂ·0.66H₂O: Elucidating the Molecular Reaction Steps by NMR Spectroscopy and Theoretical Studies. ACS Omega, 2022, 7, 5350-5365.	1.6	5
7	The Ionic Product of Water in the Eye of the Quantum Cluster Equilibrium. Molecules, 2022, 27, 1286.	1.7	6
8	Uncertainty quantification of phase transition quantities from cluster weighting calculations. Journal of Chemical Physics, 2022, 157, .	1.2	3
9	Predicting Vibrational Spectroscopy for Flexible Molecules and Molecules with Nonâ€Idle Environments. Advanced Theory and Simulations, 2021, 4, 2000223.	1.3	19
10	Influence of Complexing Additives on the Reversible Deposition/Dissolution of Magnesium in an Ionic Liquid. ChemElectroChem, 2021, 8, 390-402.	1.7	10
11	How is CO2 absorbed into a deep eutectic solvent?. Journal of Chemical Physics, 2021, 154, 094503.	1.2	28
12	Water in Protic Ionic Liquid Electrolytes: From Solvent Separated Ion Pairs to Water Clusters. ChemSusChem, 2021, 14, 3315-3324.	3.6	8
13	Molecular level insight into the solvation of cellulose in deep eutectic solvents. Journal of Chemical Physics, 2021, 155, 084501.	1.2	12
14	Calculation of improved enthalpy and entropy of vaporization by a modified partition function in quantum cluster equilibrium theory. Journal of Chemical Physics, 2021, 155, 104101.	1.2	12
15	Comparison between ab initio and polarizable molecular dynamics simulations of 1-butyl-3-methylimidazolium tetrafluoroborate and chloride in water. Journal of Molecular Liquids, 2021, 337, 116521.	2.3	14
16	Ion Pairing in Ionic Liquids. , 2021, , 1-14.		1
17	Self-aggregation of stilbazolium ion pairs in liquid chloroform. A molecular dynamics study. Journal of Molecular Liquids, 2021, 344, 117735.	2.3	1
18	TiCl4 Dissolved in Ionic Liquid Mixtures from Ðb Initio Molecular Dynamics Simulations. Molecules, 2021, 26, 79.	1.7	5

#	Article	IF	Citations
19	Non-traditional solvent effects in organic reactions. Physical Chemistry Chemical Physics, 2021, 23, 26028-26029.	1.3	3
20	Robustness of the Hydrogen Bond and Ion Pair Dynamics in Ionic Liquids to Different Parameters from the Reactive Flux Method. Journal of Chemical & Engineering Data, 2020, 65, 1146-1158.	1.0	21
21	Cluster-Weighting in Bulk Phase Vibrational Circular Dichroism. Journal of Physical Chemistry B, 2020, 124, 7272-7283.	1.2	19
22	Activity coefficients of binary methanol alcohol mixtures from cluster weighting. ChemistryOpen, 2020, 9, 774-785.	0.9	9
23	Understanding the Complex Surface Interplay for Extraction: Aâ€‰Molecular Dynamics Study. Chemistry - A European Journal, 2020, 26, 14969-14977.	1.7	1
24	Are There Magic Compositions in Deep Eutectic Solvents? Effects of Composition and Water Content in Choline Chloride/Ethylene Glycol from Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2020, 124, 7433-7443.	1.2	94
25	Glucose in dry and moist ionic liquid: vibrational circular dichroism, IR, and possible mechanisms. Physical Chemistry Chemical Physics, 2020, 22, 10726-10737.	1.3	15
26	TRAVISâ€”A free analyzer for trajectories from molecular simulation. Journal of Chemical Physics, 2020, 152, 164105.	1.2	342
27	Effect of an external electric field on the dynamics and intramolecular structures of ions in an ionic liquid. Journal of Chemical Physics, 2019, 151, 164503.	1.2	24
28	Water in Protic Ionic Liquids: Properties and Use of a New Class of Electrolytes for Energyâ€Storage Devices. ChemSusChem, 2019, 12, 3827-3836.	3.6	38
29	Strong Microheterogeneity in Novel Deep Eutectic Solvents. ChemPhysChem, 2019, 20, 1786-1792.	1.0	41
30	Tuning Solvent Miscibility: A Fundamental Assessment on the Example of Induced Methanol/n-Dodecane Phase Separation. Journal of Physical Chemistry B, 2019, 123, 4400-4407.	1.2	8
31	Anharmonicity of Vibrational Modes in Hydrogen Chlorideâ€“Water Mixtures. Journal of Chemical Theory and Computation, 2019, 15, 2535-2547.	2.3	5
32	Multifaceted Water Dynamics in Spherical Nanocages. Journal of Physical Chemistry C, 2019, 123, 5989-5998.	1.5	5
33	Understanding the fluidity of condensed phase systems in terms of voidsâ€”novel algorithm, implementation and application. Physical Chemistry Chemical Physics, 2019, 21, 4988-4997.	1.3	7
34	Interfacial Domain Formation Enhances Electrochemical Synthesis. Journal of Physical Chemistry Letters, 2019, 10, 1192-1197.	2.1	25
35	A Cluster Approach for Activity Coefficients: General Theory and Implementation. Journal of Chemical & Engineering Data, 2019, 64, 255-261.	1.0	16
36	Predicting Moleâ€Fractionâ€Dependent Dissociation for Weak Acids. Angewandte Chemie - International Edition, 2019, 58, 3212-3216.	7.2	21

#	Article	IF	Citations
37	Dissoziation schwacher SÃuren Ã¼ber den gesamten Molenbruchbereich. Angewandte Chemie, 2019, 131, 3245-3249.	1.6	11
38	Selective Electrochemical Nitrogen Reduction Driven by Hydrogen Bond Interactions at Metalâ€“Ionic Liquid Interfaces. Journal of Physical Chemistry Letters, 2019, 10, 513-517.	2.1	36
39	Cation influence on heterocyclic ammonium ionic liquids: a molecular dynamics study. Physical Chemistry Chemical Physics, 2019, 21, 4472-4486.	1.3	17
40	Finding the best density functional approximation to describe interaction energies and structures of ionic liquids in molecular dynamics studies. Journal of Chemical Physics, 2018, 148, 193835.	1.2	38
41	Thermodynamics and proton activities of protic ionic liquids with quantum cluster equilibrium theory. Journal of Chemical Physics, 2018, 148, 193822.	1.2	30
42	Structure and lifetimes in ionic liquids and their mixtures. Faraday Discussions, 2018, 206, 219-245.	1.6	74
43	Structure and dynamics of ionic liquids: general discussion. Faraday Discussions, 2018, 206, 291-337.	1.6	8
44	Ionic liquids at interfaces: general discussion. Faraday Discussions, 2018, 206, 549-586.	1.6	0
45	Peacemaker 2: Making clusters talk about binary mixtures and neat liquids. SoftwareX, 2018, 7, 356-359.	1.2	29
46	Molecular Dynamics Simulations of Lithium-Doped Ionic-Liquid Electrolytes. Journal of Physical Chemistry B, 2018, 122, 10535-10547.	1.2	28
47	Preface: Special Topic on Chemical Physics of Ionic Liquids. Journal of Chemical Physics, 2018, 148, 193501.	1.2	12
48	Hydrophilic Ionic Liquid Mixtures of Weakly and Strongly Coordinating Anions with and without Water. ACS Omega, 2018, 3, 8567-8582.	1.6	35
49	How to Harvest Grotthuss Diffusion in Protic Ionic Liquid Electrolyte Systems. ChemSusChem, 2018, 11, 1900-1910.	3.6	66
50	Vibrational signatures of anionic cyano groups in imidazolium ionic liquids. Vibrational Spectroscopy, 2017, 91, 141-146.	1.2	30
51	The Catalytic Effect of Fluoroalcohol Mixtures Depends on Domain Formation. ACS Catalysis, 2017, 7, 1846-1852.	5.5	98
52	Predicting miscibility of binary liquids from small cluster QCE calculations. Journal of Chemical Physics, 2017, 146, 154502.	1.2	19
53	Structural Investigations on Lithium-Doped Protic and Aprotic Ionic Liquids. Journal of Physical Chemistry B, 2017, 121, 5279-5292.	1.2	24
54	Effect of alkyl chain length in protic ionic liquids: an AIMD perspective. Molecular Physics, 2017, 115, 1582-1589.	0.8	20

#	Article	IF	Citations
55	Ab initio molecular dynamics simulations of SO 2 solvation in choline chloride/glycerol deep eutectic solvent. Fluid Phase Equilibria, 2017, 448, 59-68.	1.4	56
56	Theoretical Investigation of the Te₄Br₂ Molecule in Ionic Liquids. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2017, 643, 41-52.	0.6	9
57	Predicting the Ionic Product of Water. Scientific Reports, 2017, 7, 10244.	1.6	40
58	A Molecular Level Understanding of Template Effects in Ionic Liquids. Accounts of Chemical Research, 2017, 50, 2949-2957.	7.6	51
59	First examples of organosilica-based ionogels: synthesis and electrochemical behavior. Beilstein Journal of Nanotechnology, 2017, 8, 736-751.	1.5	12
60	Quantum cluster equilibrium model of N-methylformamideâ€“water binary mixtures. Journal of Chemical Physics, 2016, 144, 064305.	1.2	20
61	Can dispersion corrections annihilate the dispersion-driven nano-aggregation of non-polar groups? An ab initio molecular dynamics study of ionic liquid systems. Journal of Chemical Physics, 2016, 145, 204502.	1.2	13
62	Insights into Bulk Electrolyte Effects on the Operative Voltage of Electrochemical Double-Layer Capacitors. Journal of Physical Chemistry C, 2016, 120, 12325-12336.	1.5	15
63	Catch the carbon dioxide. Nature Chemistry, 2016, 8, 401-402.	6.6	23
64	Charge Spreading in Deep Eutectic Solvents. ChemPhysChem, 2016, 17, 3354-3358.	1.0	93
65	Ionic Liquid Induced Band Shift of Titanium Dioxide. ChemSusChem, 2016, 9, 2505-2514.	3.6	19
66	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	2.8	1
67	Tuning the Carbon Dioxide Absorption in Amino Acid Ionic Liquids. ChemSusChem, 2016, 9, 1591-1599.	3.6	47
68	Classical Magnetic Dipole Moments for the Simulation of Vibrational Circular Dichroism by ab Initio Molecular Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 509-513.	2.1	53
69	Complex Structural and Dynamical Interplay of Cyano-Based Ionic Liquids. Journal of Physical Chemistry B, 2016, 120, 2471-2483.	1.2	50
70	Computerâ€gestÃ¼tztes Design ionischer FlÃ¼ssigkeiten zur CO₂â€Absorption. Angewandte Chemie, 2015, 127, 7916-7920.	1.6	8
71	Computerâ€Aided Design of Ionic Liquids as CO₂ Absorbents. Angewandte Chemie - International Edition, 2015, 54, 7805-7809.	7.2	53
72	Domain Analysis in Nanostructured Liquids: A Postâ€Molecular Dynamics Study at the Example of Ionic Liquids. ChemPhysChem, 2015, 16, 3271-3277.	1.0	103

#	Article	IF	Citations
73	Triphilic Ionicâ€Liquid Mixtures: Fluorinated and Nonâ€fluorinated Aprotic Ionicâ€Liquid Mixtures. ChemPhysChem, 2015, 16, 3325-3333.	1.0	107
74	Ion pairing in ionic liquids. Journal of Physics Condensed Matter, 2015, 27, 463002.	0.7	108
75	Multiresolution calculation of ionic liquids. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 202-214.	6.2	108
76	Molecular features contributing to the lower viscosity of phosphonium ionic liquids compared to their ammonium analogues. Physical Chemistry Chemical Physics, 2015, 17, 20205-20216.	1.3	38
77	Adsorption Behavior of the 1,3-Dimethylimidazolium Thiocyanate and Tetracyanoborate Ionic Liquids at Anatase (101) Surface. Journal of Physical Chemistry C, 2015, 119, 15137-15149.	1.5	21
78	Stretch Out or Fold Back? Conformations of Dinuclear Gold(I) N-Heterocyclic Carbene Macrocycles. Inorganic Chemistry, 2015, 54, 6100-6111.	1.9	36
79	SO2 Solvation in the 1-Ethyl-3-Methylimidazolium Thiocyanate Ionic Liquid by Incorporation into the Extended Cationâ€“Anion Network. Journal of Solution Chemistry, 2015, 44, 838-849.	0.6	30
80	Theoretical chemistry developments: from electronic structure to simulations. Physical Chemistry Chemical Physics, 2015, 17, 14268-14269.	1.3	1
81	Toward an Accurate Modeling of Ionic Liquidâ€“TiO₂ Interfaces. Journal of Physical Chemistry C, 2015, 119, 25260-25267.	1.5	25
82	En route formation of ion pairs at the ionic liquidâ€“vacuum interface. Structural Chemistry, 2015, 26, 1343-1349.	1.0	16
83	Voronoi dipole moments for the simulation of bulk phase vibrational spectra. Physical Chemistry Chemical Physics, 2015, 17, 3207-3213.	1.3	100
84	Association in ethylammonium nitrateâ€“dimethyl sulfoxide mixtures: First structural and dynamical evidences. Journal of Non-Crystalline Solids, 2015, 407, 333-338.	1.5	27
85	Substitution effect and effect of axleâ€™s flexibility at (pseudo-)rotaxanes. Beilstein Journal of Organic Chemistry, 2014, 10, 1299-1307.	1.3	4
86	How Can a Carbene be Active in an Ionic Liquid?. Chemistry - A European Journal, 2014, 20, 1622-1629.	1.7	48
87	Interactions and structure of ionic liquids on graphene and carbon nanotubes surfaces. RSC Advances, 2014, 4, 18017-18024.	1.7	65
88	Understanding ionic liquids from theoretical methods. Journal of Molecular Liquids, 2014, 192, 71-76.	2.3	64
89	Bulk and Liquidâ€“Vapor Interface of Pyrrolidinium-Based Ionic Liquids: A Molecular Simulation Study. Journal of Physical Chemistry B, 2014, 118, 731-742.	1.2	51
90	An Abnormal Nâ€Heterocyclic Carbeneâ€“Carbon Dioxide Adduct from Imidazolium Acetate Ionic Liquids: The Importance of Basicity. Chemistry - A European Journal, 2014, 20, 13002-13008.	1.7	68

#	Article	IF	Citations
91	On the origin of ionicity in ionic liquids. Ion pairing versus charge transfer. Physical Chemistry Chemical Physics, 2014, 16, 16880-16890.	1.3	191
92	Simulating the vibrational spectra of ionic liquid systems: 1-Ethyl-3-methylimidazolium acetate and its mixtures. Journal of Chemical Physics, 2014, 141, 024510.	1.2	77
93	CO₂ Absorption in the Protic Ionic Liquid Ethylammonium Nitrate. Journal of Chemical & Engineering Data, 2014, 59, 3098-3104.	1.0	43
94	Quantum Cluster Equilibrium. Letters in Mathematical Physics, 2014, , 77-96.	0.4	7
95	Understanding the evaporation of ionic liquids using the example of 1-ethyl-3-methylimidazolium ethylsulfate. Physical Chemistry Chemical Physics, 2013, 15, 18424.	1.3	30
96	Side chain fluorination and anion effect on the structure of 1-butyl-3-methylimidazolium ionic liquids. Journal of Chemical Physics, 2013, 139, 084502.	1.2	63
97	Dynamics at a Janus Interface. Journal of Physical Chemistry C, 2013, 117, 4561-4567.	1.5	20
98	Significant Cation Effects in Carbon Dioxideâ€“Ionic Liquid Systems. ChemPhysChem, 2013, 14, 315-320.	1.0	77
99	Computing vibrational spectra from ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2013, 15, 6608.	1.3	414
100	Carbene Formation in Ionic Liquids: Spontaneous, Induced, or Prohibited?. Journal of Physical Chemistry B, 2013, 117, 5898-5907.	1.2	109
101	Liquid Structure and Cluster Formation in Ionic Liquid/Water Mixtures â€“ An Extensive ab initio Molecular Dynamics Study on 1-Ethyl-3-Methylimidazolium Acetate/Water Mixtures â€“ Part. Zeitschrift Fur Physikalische Chemie, 2013, 227, 177-204.	1.4	48
102	A one-parameter quantum cluster equilibrium approach. Journal of Chemical Physics, 2012, 137, 164107.	1.2	11
103	Performance of dispersion-corrected density functional theory for the interactions in ionic liquids. Physical Chemistry Chemical Physics, 2012, 14, 4875.	1.3	202
104	The bulk and the gas phase of 1-ethyl-3-methylimidazolium ethylsulfate: dispersion interaction makes the difference. Physical Chemistry Chemical Physics, 2012, 14, 12079.	1.3	42
105	Using Molecular Simulation to Understand the Structure of [C₂C₁im]⁺â€“Alkylsulfate Ionic Liquids: Bulk and Liquidâ€“Vapor Interfaces. Journal of Physical Chemistry B, 2012, 116, 14159-14170.	1.2	31
106	On the ideality of binary mixtures of ionic liquids. Physical Chemistry Chemical Physics, 2012, 14, 13204.	1.3	90
107	Proton transfer and polarity changes in ionic liquidâ€“water mixtures: a perspective on hydrogen bonds from ab initio molecular dynamics at the example of 1-ethyl-3-methylimidazolium acetateâ€“water mixturesâ€”Part 1. Physical Chemistry Chemical Physics, 2012, 14, 5030.	1.3	144
108	Short Time Dynamics of Ionic Liquids in AIMD-Based Power Spectra. Journal of Chemical Theory and Computation, 2012, 8, 1570-1579.	2.3	70

#	Article	IF	Citations
109	From molten salts to room temperature ionic liquids: Simulation studies on chloroaluminate systems. Faraday Discussions, 2012, 154, 171-188.	1.6	59
110	Effect of Dispersion on the Structure and Dynamics of the Ionic Liquid 1â€Ethylâ€3â€methylimidazolium Thiocyanate. ChemPhysChem, 2012, 13, 1845-1853.	1.0	81
111	Coupled Cluster in Condensed Phase. Part II: Liquid Hydrogen Fluoride from Quantum Cluster Equilibrium Theory. Journal of Chemical Theory and Computation, 2011, 7, 868-875.	2.3	33
112	Coupled Cluster in Condensed Phase. Part I: Static Quantum Chemical Calculations of Hydrogen Fluoride Clusters. Journal of Chemical Theory and Computation, 2011, 7, 843-851.	2.3	39
113	Depolarization of water in protic ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 15083.	1.3	63
114	Ab initio molecular dynamics simulations of a binary system of ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 13617.	1.3	69
115	Binary systems from quantum cluster equilibrium theory. Journal of Chemical Physics, 2011, 135, 194113.	1.2	44
116	How Hydrogen Bonds Influence the Mobility of Imidazolium-Based Ionic Liquids. A Combined Theoretical and Experimental Study of 1-n-Butyl-3-methylimidazolium Bromide. Journal of Physical Chemistry B, 2011, 115, 15280-15288.	1.2	118
117	Performance of Quantum Chemically Derived Charges and Persistence of Ion Cages in Ionic Liquids. A Molecular Dynamics Simulations Study of 1-n-Butyl-3-methylimidazolium Bromide. Journal of Physical Chemistry B, 2011, 115, 693-702.	1.2	137
118	Real-World Predictions from Ab Initio Molecular Dynamics Simulations. Topics in Current Chemistry, 2011, 307, 109-153.	4.0	89
119	TRAVIS - A Free Analyzer and Visualizer for Monte Carlo and Molecular Dynamics Trajectories. Journal of Chemical Information and Modeling, 2011, 51, 2007-2023.	2.5	930
120	Locality and Fluctuations: Trends in Imidazolium-Based Ionic Liquids and Beyond. Journal of Chemical Theory and Computation, 2011, 7, 3040-3044.	2.3	93
121	Nitrile-Functionalized Pyridinium, Pyrrolidinium, and Piperidinium Ionic Liquids. Journal of Physical Chemistry B, 2011, 115, 8424-8438.	1.2	58
122	What can clusters tell us about the bulk?. Computer Physics Communications, 2011, 182, 1428-1446.	3.0	46
123	Importance of Structural Motifs in Liquid Hydrogen Fluoride. ChemPhysChem, 2011, 12, 3474-3482.	1.0	31
124	Comparison of Free Energy Surfaces Calculations from Ab Initio Molecular Dynamic Simulations at the Example of Two Transition Metal Catalyzed Reactions. International Journal of Molecular Sciences, 2011, 12, 1389-1409.	1.8	12
125	Towards a Molecular Understanding of Cationâ€“Anion Interactionsâ€”Probing the Electronic Structure of Imidazolium Ionic Liquids by NMR Spectroscopy, Xâ€ray Photoelectron Spectroscopy and Theoretical Calculations. Chemistry - A European Journal, 2010, 16, 9018-9033.	1.7	264
126	The role of hydrogen atoms in interactions involving imidazolium-based ionic liquids. Journal of Molecular Structure, 2010, 972, 22-34.	1.8	141

#	Article	IF	Citations
127	Theoretical Investigation of Solvent Effects and Complex Systems: Toward the calculations of bioinorganic systems from ab initio molecular dynamics simulations and static quantum chemistry. Advances in Inorganic Chemistry, 2010, 62, 111-142.	0.4	9
128	Structure and dynamics of the protic ionic liquid monomethylammonium nitrate ([CH3NH3][NO3]) from ab initio molecular dynamics simulations. Journal of Chemical Physics, 2010, 132, 124506.	1.2	111
129	Estimating the Hydrogen Bond Energy. Journal of Physical Chemistry A, 2010, 114, 9529-9536.	1.1	291
130	On the physical origin of the cationâ€“anion intermediate bond in ionic liquids Part I. Placing a (weak) hydrogen bond between two charges. Physical Chemistry Chemical Physics, 2010, 12, 7473.	1.3	124
131	Uncovering Individual Hydrogen Bonds in Rotaxanes by Frequency Shifts. Journal of the American Chemical Society, 2010, 132, 484-494.	6.6	19
132	Quantum Cluster Equilibrium Theory Applied in Hydrogen Bond Number Studies of Water. 1. Assessment of the Quantum Cluster Equilibrium Model for Liquid Water. Journal of Chemical Theory and Computation, 2009, 5, 1640-1649.	2.3	34
133	Quantum Cluster Equilibrium Theory Applied in Hydrogen Bond Number Studies of Water. 2. Icebergs in a Two-Dimensional Water Continuum?. Journal of Chemical Theory and Computation, 2009, 5, 1650-1656.	2.3	27
134	Unexpected Hydrogen Bond Dynamics in Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 15129-15132.	1.2	112
135	Are There Stable Ion-Pairs in Room-Temperature Ionic Liquids? Molecular Dynamics Simulations of 1-n-Butyl-3-methylimidazolium Hexafluorophosphate. Journal of the American Chemical Society, 2009, 131, 15825-15833.	6.6	283
136	How Can Rotaxanes Be Modified by Varying Functional Groups at the Axle?â€"A Combined Theoretical and Experimental Analysis of Thermochemistry and Electronic Effects. Chemistry - A European Journal, 2008, 14, 1216-1227.	1.7	19
137	Intermolecular Forces in an Ionic Liquid ([Mmim][Cl]) versus Those in a Typical Salt (NaCl). Angewandte Chemie - International Edition, 2008, 47, 3639-3641.	7.2	174
138	Theoretical energetic and vibrational analysis of amide-templated pseudorotaxanes. Chemical Physics, 2008, 343, 186-199.	0.9	9
139	Ionic Liquids from Theoretical Investigations. Topics in Current Chemistry, 2008, 290, 213-262.	4.0	74
140	What keeps ionic liquids in flow?. Physical Chemistry Chemical Physics, 2008, 10, 6921.	1.3	130
141	Why are ionic liquid ions mainly associated in water? A Carâ€“Parrinello study of 1-ethyl-3-methyl-imidazolium chloride water mixture. Journal of Chemical Physics, 2008, 129, 104505.	1.2	130
142	When Is a Molecule Properly Solvated by a Continuum Model or in a Cluster Ansatz? A First-Principles Simulation of Alanine Hydration. Journal of Physical Chemistry B, 2008, 112, 1456-1464.	1.2	38
143	Validation of Dispersion-Corrected Density Functional Theory Approaches for Ionic Liquid Systems. Journal of Physical Chemistry A, 2008, 112, 8430-8435.	1.1	113
144	First-Principles Investigation of the Schrock Mechanism of Dinitrogen Reduction Employing the Full HIPTN₃N Ligand. Inorganic Chemistry, 2008, 47, 3634-3650.	1.9	111

#	Article	IF	Citations
145	Introducing phase transitions to quantum chemistry: From Troutonâ€™s rule to first principles vaporization entropies. Journal of Chemical Physics, 2008, 128, 244506.	1.2	23
146	Green Chemistry from Supercomputers: Car-Parrinello Simulations of Emim-Chloroaluminates Ionic Liquids. , 2008, , 213-227.		1
147	Green Chemistry from Supercomputers: Carâ€“Parrinello Simulations of Emim-Chloroaluminates Ionic Liquids. , 2008, , 157-171.		0
148	The Structure of Imidazolium-Based Ionic Liquids: Insights From Ion-Pair Interactions. Australian Journal of Chemistry, 2007, 60, 9.	0.5	199
149	Choline Saccharinate and Choline Acesulfamate:Â Ionic Liquids with Low Toxicities. Journal of Physical Chemistry B, 2007, 111, 5254-5263.	1.2	224
150	Ionic Liquids from Carâ˜Parrinello Simulations. 2. Structural Diffusion Leading to Large Anions in Chloraluminate Ionic Liquids. Inorganic Chemistry, 2007, 46, 2751-2754.	1.9	53
151	Basis Set Superposition Error along the Free-Energy Surface of the Water Dimer. Journal of Chemical Theory and Computation, 2007, 3, 1510-1517.	2.3	4
152	Eigen or Zundel Ion: News from Calculated and Experimental Photoelectron Spectroscopy. ChemPhysChem, 2007, 8, 41-43.	1.0	42
153	Theoretical bioinorganic chemistry: the electronic structure makes a difference. Current Opinion in Chemical Biology, 2007, 11, 134-141.	2.8	141
154	Theory of complicated liquidsInvestigation of liquids, solvents and solvent effects with modern theoretical methods. Physics Reports, 2007, 440, 1-111.	10.3	67
155	Green Chemistry from Supercomputers: Car-Parrinello Simulations for Ionic Liquids. , 2007, , 135-144.		0
156	Cooperativity in ionic liquids. Journal of Chemical Physics, 2006, 124, 174506.	1.2	153
157	Task-Specific Ionic Liquid for Solubilizing Metal Oxides. Journal of Physical Chemistry B, 2006, 110, 20978-20992.	1.2	412
158	Frequency Analysis of Amide-Linked Rotaxane Mimetics. Journal of Physical Chemistry A, 2006, 110, 12963-12970.	1.1	22
159	Hydrogen Bond Detection. Journal of Physical Chemistry A, 2006, 110, 4229-4237.	1.1	62
160	Surface redox chemistry of adsorbed viologens on Cu(100). New Journal of Chemistry, 2006, 30, 1439-1451.	1.4	40
161	Density functional embedding for molecular systems. Chemical Physics Letters, 2006, 421, 16-20.	1.2	84
162	Ionic Liquids from Carâ˜Parrinello Simulations, Part I:Â Liquid AlCl3. Journal of Physical Chemistry B, 2006, 110, 11475-11480.	1.2	31

#	Article	IF	Citations
163	Characterising the Electronic Structure of Ionic Liquids: An Examination of the 1-Butyl-3-Methylimidazolium Chloride Ion Pair. Chemistry - A European Journal, 2006, 12, 6762-6775.	1.7	427
164	Carâ€“Parrinello Molecular Dynamics Simulations and Biological Systems. , 2006, , 133-171.		20
165	Car-Parrinello Molecular Dynamics Study of the Initial Dinitrogen Reduction Step in Sellmann-Type Nitrogenase Model Complexes. Chemistry - A European Journal, 2005, 11, 574-583.	1.7	31
166	Nitrogen Fixation under Mild Ambient Conditions: Part Iâ€”The Initial Dissociation/Association Step at Molybdenum Triamidoamine Complexes. Chemistry - A European Journal, 2005, 11, 7448-7460.	1.7	71
167	Cooperative versus dispersion effects: What is more important in an associated liquid such as water?. Journal of Chemical Physics, 2005, 123, 204116.	1.2	62
168	Understanding the Template Preorganization Step of an Artificial Arginine ReceptorÂ§. Journal of the American Chemical Society, 2005, 127, 8748-8756.	6.6	14
169	Solvent effects on electronic properties from Wannier functions in a dimethyl sulfoxide/water mixture. Journal of Chemical Physics, 2004, 121, 5133-5142.	1.2	89
170	HYDROPHOBIC HYDRATION FROM CARâ€“PARRINELLO SIMULATIONS. International Journal of Modern Physics B, 2004, 18, 1951-1962.	1.0	29
171	A Photochemical Activation Scheme of Inert Dinitrogen by Dinuclear RuII and FeII Complexes. Chemistry - A European Journal, 2004, 10, 4443-4453.	1.7	48
172	Visualizing Degrees of Aromaticity for Different Barbaralane Systems. Journal of Physical Chemistry A, 2004, 108, 11728-11732.	1.1	21
173	s-Tetrazine in Aqueous Solution:Â A Density Functional Study of Hydrogen Bonding and Electronic Excitations. Journal of Physical Chemistry A, 2004, 108, 2044-2052.	1.1	33
174	A Wavefunction-Based Criterion for the Detection of Intermolecular Interactions in Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2003, 107, 4141-4146.	1.1	21
175	Fast Anomalous Diffusion of Small Hydrophobic Species in Water. Physical Review Letters, 2002, 89, 215901.	2.9	50
176	The Secret of Dimethyl Sulfoxideâ^'Water Mixtures. A Quantum Chemical Study of 1DMSOâ^'nWater Clusters. Journal of the American Chemical Society, 2002, 124, 6206-6215.	6.6	174
177	Is there an iceberg effect in the water/DMSO mixture? Some information from computational chemistry. Journal of Molecular Liquids, 2002, 98-99, 71-77.	2.3	7
178	The structure of a DMSOâ€“water mixture from Carâ€“Parrinello simulations. Chemical Physics Letters, 2002, 364, 497-502.	1.2	61
179	Disproving the Iceberg Effect? A Study of the Deuteron Quadrupole Coupling Constant of Water in a Mixture with Dimethyl Sulfoxide via Computer Simulations. Journal of the American Chemical Society, 2000, 122, 5379-5383.	6.6	31
180	Calculation of bulk properties of liquids and supercritical fluids from pure theory. Chemical Society Reviews, 1999, 28, 121-133.	18.7	46

#	Article	IF	Citations
181	Chemical Accuracy Obtained in an Ab Initio Molecular Dynamics Simulation of a Fluid by Inclusion of a Three-Body Potential. Chemistry - A European Journal, 1998, 4, 383-388.	1.7	31
182	Melting curves for neon calculated from pure theory. Journal of Chemical Physics, 1998, 108, 4107-4111.	1.2	70
183	Theoretical Methods for Supramolecular Chemistry. , 0, , 419-471.		0
184	Uncovering molecular secrets of ionic liquids. Chemical Modelling, 0, , 1-24.	0.2	10