Bernd M Rode

List of Publications by Year
in descending order

240 papers	8,117 citations	47006 47 h-index	85541 71 g-index
244 all docs	244 docs citations	244 times ranked	3922 citing authors

#	Article	IF	Citations
1	Characterization of dynamics and reactivities of solvated ions byab initio simulations. Journal of Computational Chemistry, 2004, 25, 211-217.	3.3	261
2	Bornâ˜'Oppenheimer ab Initio QM/MM Dynamics Simulations of Na+and K+in Water:Â From Structure Making to Structure Breaking Effects. Journal of Physical Chemistry A, 1998, 102, 10340-10347.	2.5	218
3	Ab initio quantum mechanical charge field (QMCF) molecular dynamics: a QM/MM â€“ MD procedure for accurate simulations of ions and complexes. Theoretical Chemistry Accounts, 2006, 115, 77-85.	1.4	183
4	A QM/MM simulation method applied to the solution of Li+ in liquid ammonia. Chemical Physics, 1996, 211, 313-323.	1.9	175
5	Solvation of Ca2+in Water Studied by Bornâ˜'Oppenheimer ab Initio QM/MM Dynamics. Journal of Physical Chemistry A, 1997, 101, 6299-6309.	2.5	140
6	Molecular dynamics simulations of Ca2+ in water: Comparison of a classical simulation including three-body corrections and Bornâ€“Oppenheimer ab initio and density functional theory quantum mechanical/molecular mechanics simulations. Journal of Chemical Physics, 2001, 115, 10808-10813.	3.0	140
7	The hydration structure of the lithium ion. Journal of Chemical Physics, 2002, 117, 110-117.	3.0	133
8	Structure and Dynamics of Sulfate Ion in Aqueous SolutionAnab initioQMCF MD Simulation and Large Angle X-ray Scattering Study. Journal of Physical Chemistry B, 2007, 111, 4150-4155.	2.6	116
9	Structure and ultrafast dynamics of liquid water: A quantum mechanics/molecular mechanics molecular dynamics simulations study. Journal of Chemical Physics, 2005, 122, 174506.	3.0	106
10	Extendedab initioquantum mechanical/molecular mechanical molecular dynamics simulations of hydrated Cu2+. Journal of Chemical Physics, 2003, 119, 9523-9531.	3.0	97
11	Structure and dynamics of hydrated ionsâ€"new insights through quantum mechanical simulations. Journal of Molecular Liquids, 2004, 110, 105-122.	4.9	94
12	â€œStructure Breakingâ€•Effect of Hydrated Cs+. Journal of Physical Chemistry A, 2004, 108, 1509-1514.	2.5	93
13	Possible Role of Copper and Sodium Chloride in Prebiotic Evolution of Peptides. Analytical Sciences, 1989, 5, 411-414.	1.6	91
14	New Insights into the Jahn-Teller Effect through ab initio Quantum-Mechanical/Molecular-Mechanical Molecular Dynamics Simulations of CuII in Water. ChemPhysChem, 2003, 4, 931-943.	2.1	91
15	The Structure of Liquid Formamide Studied by Means of X-Ray Diffraction andab InitioLCGO-MO-SCF Calculations. Bulletin of the Chemical Society of Japan, 1983, 56, 2116-2121.	3.2	90
16	The hydration shell structure of Li+ investigated by Bornâ€“Oppenheimer ab initio QM/MM dynamics. Chemical Physics Letters, 1998, 286, 56-64.	2.6	89
17	Silica, Alumina, and Clay-Catalyzed Alanine Peptide Bond Formation. Journal of Molecular Evolution, 1997, 45, 457-466.	1.8	83
18	Juliflorine: A potent natural peripheral anionic-site-binding inhibitor of acetylcholinesterase with calcium-channel blocking potential, a leading candidate for Alzheimerâ€™s disease therapy. Biochemical and Biophysical Research Communications, 2005, 332, 1171-1179.	2.1	83

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19	Silica, alumina and clay catalyzed peptide bond formation: enhanced efficiency of alumina catalyst. , 1999, 29, 451-461.		81
20	Hydration of Sodium(I) and Potassium(I) Revisited: A Comparative QM/MM and QMCF MD Simulation Study of Weakly Hydrated Ions. Journal of Physical Chemistry A, 2009, 113, 1827-1834.	2.5	78
21	Ab Initio Quantum Mechanical Charge Field Molecular Dynamicsâ€"A Nonparametrized First-Principle Approach to Liquids and Solutions. Advances in Quantum Chemistry, 2010, , 213-246.	0.8	76
22	The effect of smectite composition on the catalysis of peptide bond formation. Journal of Molecular Evolution, 1996, 43, 326-333.	1.8	69
23	Investigation of Cu2+ Hydration and the Jahnâ˜Teller Effect in Solution by QM/MM Monte Carlo Simulations. Journal of Physical Chemistry A, 1999, 103, 11387-11393.	2.5	69
24	The Structure of LiquidN-Methylformamide by Means of X-Ray Diffraction and Ab Initio LCGOâ€"MOâ€"SCF Calculations. Bulletin of the Chemical Society of Japan, 1986, 59, 271-276.	3.2	67
25	Copper-catalyzed amino acid condensation in water â€" A simple possible way of prebiotic peptide formation. Origins of Life and Evolution of Biospheres, 1990, 20, 401-410.	1.9	67
26	The combination of salt induced peptide formation reaction and clay catalysis: a way to higher peptides under primitive earth conditions. Origins of Life and Evolution of Biospheres, 1999, 29, 273-286.	1.9	66
27	An extended ab initio QM/MM MD approach to structure and dynamics of Zn(II) in aqueous solution. Journal of Chemical Physics, 2005, 123, 054514.	3.0	65
28	Structure and dynamics of phosphate ion in aqueous solution: An ab initio QMCF MD study. Journal of Computational Chemistry, 2008, 29, 2330-2334.	3.3	64
29	Peptide chain elongation: A possible role of montmorillonite in prebiotic synthesis of protein precursors. Origins of Life and Evolution of Biospheres, 1995, 25, 431-441.	1.9	62
30	Hydration Structure and Water Exchange Reaction of Nickel(II) Ion:Â Classical and QM/MM Simulations. Journal of Physical Chemistry A, 2002, 106, 6783-6791.	2.5	62
31	Structure and Dynamics of Metal Ions in Solution:â€‰ QM/MM Molecular Dynamics Simulations of Mn2+ and V2+. Journal of the American Chemical Society, 2003, 125, 1618-1624.	13.7	60
32	Structure and dynamics of liquid formamide. Chemical Physics, 1995, 190, 61-82.	1.9	57
33	Predictions of rate constants and estimates for tunneling splittings of concerted proton transfer in small cyclic water clusters. Journal of Chemical Physics, 1998, 109, 2672-2679.	3.0	57
34	How to access structure and dynamics of solutions: The capabilities of computational methods (Special Topic Article). Pure and Applied Chemistry, 2006, 78, 525-539.	1.9	57
35	Amino acids on the rampant primordial Earth: Electric discharges and the hot salty ocean. Molecular Diversity, 2006, 10, 3-7.	3.9	57
36	Evaporation cycle experiments â€" A simulation of salt-induced peptide synthesis under possible prebiotic conditions. Origins of Life and Evolution of Biospheres, 1993, 23, 167-176.	1.9	56

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37	Simulations of Liquids and Solutions Based on Quantum Mechanical Forces. Advances in Inorganic Chemistry, 2010, 62, 143-175.	1.0	56
38	Monte Carlo Simulations of Zn(II) in Water Including Three-Body Effects. The Journal of Physical Chemistry, 1996, 100, 6808-6813.	2.9	54
39	Librational, vibrational, and exchange motions of water molecules in aqueous Ni(II) solution: classical and QM/MM molecular dynamics simulations. Chemical Physics Letters, 2002, 358, 449-458.	2.6	53
40	Structure and Dynamics of Solvated Sn(II) in Aqueous Solution:Â An ab Initio QM/MM MD Approach. Journal of the American Chemical Society, 2005, 127, 14231-14238.	13.7	53
41	The effect of clay structure on peptide bond formation catalysis. Journal of Molecular Catalysis A, 1999, 144, 129-136.	4.8	52
42	Structure and Dynamics of Hydrated Ag (I): Ab Initio Quantum Mechanical-Molecular Mechanical Molecular Dynamics Simulation. Journal of Physical Chemistry A, 2003, 107, 3132-3138.	2.5	52
43	Structure and dynamics of the hydrated palladium(II) ion in aqueous solution A QMCF MD simulation and EXAFS spectroscopic study. Chemical Physics Letters, 2007, 445, 193-197.	2.6	51
44	Glycine and diglycine as possible catalytic factors in the prebiotic evolution of peptides. Origins of Life and Evolution of Biospheres, 2002, 32, 225-236.	1.9	50
45	Dynamics of the solvation process of Ca2+ in water. Chemical Physics Letters, 2001, 349, 99-103.	2.6	49
46	QM/MM Molecular Dynamics Simulation of the Structure of Hydrated Fe(II) and Fe(III) Ions. Journal of Physical Chemistry A, 2003, 107, 2324-2328.	2.5	49
47	Influence of Electron Correlation Effects on the Solvation of Cu2+. Journal of the American Chemical Society, 2004, 126, 12786-12787.	13.7	49
48	Sr(II) in Water:Â A Labile Hydrate with a Highly Mobile Structure. Journal of Physical Chemistry B, 2006, 110, 20409-20417.	2.6	49
49	Influence of polarization and many body quantum effects on the solvation shell of Al(iii) in dilute aqueous solutionâ€"extended ab initio QM/MM MD simulations. Physical Chemistry Chemical Physics, 2005, 7, 1382-1387.	2.8	48
50	A Quantum Mechanical Charge Field Molecular Dynamics Study of Fe²⁺ and Fe³⁺ Ions in Aqueous Solutions. Inorganic Chemistry, 2010, 49, 5101-5106.	4.0	48
51	Symmetry Breaking and Hydration Structure of Carbonate and Nitrate in Aqueous Solutions: A Study by Ab Initio Quantum Mechanical Charge Field Molecular Dynamics. Journal of Physical Chemistry B, 2011, 115, 12527-12536.	2.6	48
52	Hydration of highly charged ions. Chemical Physics Letters, 2011, 512, 139-145.	2.6	48
53	Salt induced peptide formation: on the selectivity of the copper induced peptide formation under possible prebiotic conditions. Inorganica Chimica Acta, 1995, 228, 207-214.	2.4	47
54	Structure and dynamics of solvated Ba(II) in dilute aqueous solution â€“ an ab initio QM/MM MD approach. Chemical Physics, 2005, 312, 81-88.	1.9	47

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55	The First Steps of Chemical Evolution towards the Origin of Life. Chemistry and Biodiversity, 2007, 4, 2674-2702.	2.1	47
56	Glycine oligomerization on silica and alumina. Reaction Kinetics and Catalysis Letters, 1997, 62, 281-286.	0.6	46
57	The solvation structure of Pb(II) in dilute aqueous solution: An ab initio quantum mechanical/molecular mechanical molecular dynamics approach. Journal of Chemical Physics, 2004, 121, 6406-6411.	3.0	46
58	Structure and Dynamics of the U⁴⁺ Ion in Aqueous Solution: An ab Initio Quantum Mechanical Charge Field Molecular Dynamics Study. Inorganic Chemistry, 2009, 48, 3993-4002.	4.0	46
59	Salt-induced formation of mixed peptides under possible prebiotic conditions. Inorganica Chimica Acta, 1991, 186, 247-251.	2.4	45
60	Structure-breaking effects of solvated Rb(I) in dilute aqueous solutionâ€"Anab initio QM/MM MD approach. Journal of Computational Chemistry, 2005, 26, 949-956.	3.3	45
61	Classical and Mixed Quantum Mechanical/Molecular Mechanical Simulation of Hydrated Manganous Ion. Journal of Physical Chemistry A, 2001, 105, 7646-7650.	2.5	44
62	Structure and Dynamics of the UO₂²⁺ Ion in Aqueous Solution: An Ab Initio QMCF MD Study. Journal of Physical Chemistry A, 2009, 113, 12496-12503.	2.5	44
63	Chemical evolution from simple inorganic compounds to chiral peptides. Chemical Society Reviews, 2012, 41, 5484.	38.1	44
64	Reaction-Path Dynamics of Hydroxyl Radical Reactions with Ethane and Haloethanes. Journal of Physical Chemistry A, 1997, 101, 4245-4253.	2.5	43
65	Al(III) Hydration Revisited. An ab Initio Quantum Mechanical Charge Field Molecular Dynamics Study. Journal of Physical Chemistry B, 2008, 112, 11726-11733.	2.6	43
66	A new type of metal chelate affinity chromatography using trivalent lanthanide ions for phosphopeptide enrichment. Analyst, The, 2013, 138, 2995.	3.5	43
67	Dynamics in the hydration shell of Hg2+ ion: classical and ab initio QM/MM molecular dynamics simulations. Chemical Physics Letters, 2003, 371, 438-444.	2.6	42
68	Molecular Docking Studies of Natural Cholinesterase-Inhibiting Steroidal Alkaloids fromSarcococcasaligna. Journal of Medicinal Chemistry, 2003, 46, 5087-5090.	6.4	42
69	Beryllium(II): The Strongest Structure-Forming Ion in Water? A QMCF MD Simulation Study. Journal of Physical Chemistry B, 2009, 113, 9289-9295.	2.6	39
70	Monte-Carlo Simulations of Cu(II) in Water with 3-Body Potential. The Journal of Physical Chemistry, 1995, 99, 15714-15717.	2.9	38
71	Revisiting the Hydration of Pb(II): A QMCF MD Approach. Journal of Physical Chemistry B, 2009, 113, 13007-13013.	2.6	38
72	Investigations on the mechanism of the salt-induced peptide formation. Origins of Life and Evolution of Biospheres, 1992, 22, 349-359.	1.9	37

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73	New Insights into the Dynamics of Concerted Proton Tunneling in Cyclic Water and Hydrogen Fluoride Clusters. Journal of Physical Chemistry A, 1997, 101, 4707-4716.	2.5	37
74	Dynamical properties of the water molecules in the hydration shells of Fe(II) and Fe(III) ions: ab initio QM/MM molecular dynamics simulations. Chemical Physics Letters, 2003, 367, 586-592.	2.6	37
75	Structure and Dynamics of Au+Ion in Aqueous Solution: Ab Initio QM/MM MD Simulations. Journal of the American Chemical Society, 2004, 126, 2582-2587.	13.7	37
76	Catalysis of dialanine formation by glycine in the salt-induced peptide formation reaction. , 1998, 28, 79-90.		36
77	Stereoselective differentiation in the Salt-induced Peptide Formation reaction and its relevance for the origin of life. Peptides, 2005, 26, 535-541.	2.4	36
78	Quantum mechanical simulation studies of molecular vibrations and dynamics of oxo-anions in water. Chemical Physics, 2008, 346, 182-185.	1.9	36
79	Local density corrected three-body distribution functions for probing local structure reorganization in liquids. Physical Chemistry Chemical Physics, 2008, 10, 6653.	2.8	36
80	Structural and Dynamical Properties and Vibrational Spectra of Bisulfate Ion in Water: A Study by Ab Initio Quantum Mechanical Charge Field Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 11561-11569.	2.6	36
81	Selective enrichment of phosphopeptides by a metalâ€“organic framework. Analytical Methods, 2013, 5, 2379.	2.7	36
82	Zinc ion in water: intermolecular potential with approximate three-body correction and Monte Carlo simulation. Chemical Physics, 1991, 156, 403-412.	1.9	35
83	Influence of heteroligands on structural and dynamical properties of hydrated Cu2+: QM/MM MD simulations. Physical Chemistry Chemical Physics, 2003, 5, 3418.	2.8	35
84	Ab initio calculations concerning the reaction mechanism of the copper(II) catalyzed glycine condensation in aqueous sodium chloride solution. Chemical Physics Letters, 1992, 197, 181-186.	2.6	34
85	Investigation on the mechanism of peptide chain prolongation on montmorillonite. Journal of Inorganic Biochemistry, 1996, 61, 69-78.	3.5	34
86	Solvation of Cu2+ in Liquid Ammonia:â€‰ Monte Carlo Simulation Including Three-Body Corrections. Journal of Physical Chemistry A, 1999, 103, 4298-4302.	2.5	34
87	Structure and dynamics of La(III) in aqueous solution â€“ An ab initio QM/MM MD approach. Chemical Physics, 2006, 327, 31-42.	1.9	34
88	The hydrated platinum(ii) ion in aqueous solutionâ€”a combined theoretical and EXAFS spectroscopic study. Dalton Transactions, 2009, , 1512.	3.3	34
89	Selective adsorption and chiral amplification of amino acids in vermiculite clay-implications for the origin of biochirality. Physical Chemistry Chemical Physics, 2011, 13, 831-838.	2.8	34
90	Molecular dynamics simulations of aqueous formamide solution. II. Dynamics of solvent molecules. Journal of Chemical Physics, 1995, 102, 2920-2927.	3.0	33

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91	Preferential Solvation of Li+ in 18.45 Aqueous Ammonia:â€‰ A Bornâ€“Oppenheimer ab Initio Quantum Mechanics/Molecular Mechanics MD Simulation. Journal of Physical Chemistry A, 1999, 103, 8524-8527.	2.5	32
92	Molecular dynamics simulations of Hg2+ in aqueous solution includingN-body effects. Journal of Chemical Physics, 2003, 118, 5065-5070.	3.0	32
93	Indications towards a stereoselectivity of the salt-induced peptide formation reaction. Inorganica Chimica Acta, 2004, 357, 649-656.	2.4	32
94	Amino acid sequence preferences of the salt-induced peptide formation reaction in comparison to archaic cell protein composition. Inorganica Chimica Acta, 1997, 254, 309-314.	2.4	31
95	3D-QSAR Studies on natural acetylcholinesterase inhibitors of Sarcococca saligna by comparative molecular field analysis (CoMFA). Bioorganic and Medicinal Chemistry Letters, 2003, 13, 4375-4380.	2.2	31
96	Structure and dynamics of the Cr(III) ion in aqueous solution:Ab initio QM/MM molecular dynamics simulation. Journal of Computational Chemistry, 2004, 25, 1576-1583.	3.3	31
97	On the structure and dynamics of the hydrated sulfite ion in aqueous solution â€“ an ab initio QMCF MD simulation and large angle X-ray scattering study. Dalton Transactions, 2012, 41, 5209.	3.3	31
98	Salt-induced peptide formation from amino acids in the presence of clays and related catalysts. Inorganica Chimica Acta, 1998, 272, 89-94.	2.4	30
99	Molecular Dynamics Simulations of the Hydrated Trivalent Transition Metal Ions Ti3+, Cr3+, and Co3+. Journal of Physical Chemistry A, 2002, 106, 10584-10589.	2.5	30
100	Structure and Dynamics of the Cd2+ Ion in Aqueous Solution:â€‰ Ab Initio QM/MM Molecular Dynamics Simulation. Journal of Physical Chemistry A, 2003, 107, 10330-10334.	2.5	30
101	The Jahn-Teller Effect of the TiIII Ion in Aqueous Solution: Extended Ab Initio QM/MM Molecular Dynamics Simulations. ChemPhysChem, 2004, 5, 1499-1506.	2.1	30
102	Large Curvature Tunneling Effects Reveal Concerted Hydrogen Exchange Rates in Cyclic Hydrogen Fluoride Clusters Comparable to Carboxylic Acid Dimers. Journal of the American Chemical Society, 1998, 120, 404-412.	13.7	29
103	Mutual amino acid catalysis in salt-induced peptide formation supports this mechanism's role in prebiotic peptide evolution. , 1999, 29, 463-471.		29
104	Structure and dynamics of the Zr⁴⁺ion in water. Physical Chemistry Chemical Physics, 2011, 13, 224-229.	2.8	29
105	What Is the Solvation Number of Na+ in Ammonia? An Ab Initio QM/MM Molecular Dynamics Study. Journal of Physical Chemistry A, 2000, 104, 7073-7078.	2.5	28
106	Solvation energy and vibrational spectrum of sulfate in water â€“ An ab initio quantum mechanical simulation. Chemical Physics Letters, 2007, 443, 152-157.	2.6	28
107	The stability of [Zn(NH3)4]2+ in water: A quantum mechanical/molecular mechanical molecular dynamics study. Physical Chemistry Chemical Physics, 2010, 12, 9713.	2.8	28
108	Are prions a relic of an early stage of peptide evolution?â˜†. Peptides, 1999, 20, 1513-1516.	2.4	27

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109	Catalytic effects of histidine enantiomers and glycine on the formation of dileucine and dimethionine in the salt-induced peptide formation reaction. Amino Acids, 2010, 38, 287-294.	2.7	27
110	Monte Carlo Simulations with an Improved Potential Function for Cu(II)-Water Including Neighbour Ligand Corrections. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1991, 46, 357-362.	1.5	26
111	Zinc(II) in liquid ammonia: Intermolecular potential including threeâ€body terms and Monte Carlo simulation. Journal of Chemical Physics, 1992, 96, 6945-6949.	3.0	26
112	The effect of reaction conditions on montmorillonite-catalysed peptide formation. Catalysis Letters, 1996, 37, 267-272.	2.6	26
113	Molecular dynamics simulation of the hydration of transition metal ions: the role of non-additive effects in the hydration shells of Fe2+ and Fe3+ ions. Chemical Physics Letters, 2004, 385, 491-497.	2.6	26
114	Cuii in Liquid Ammonia: An Approach by Hybrid Quantum-Mechanical/Molecular-Mechanical Molecular Dynamics Simulation. ChemPhysChem, 2004, 5, 342-348.	2.1	26
115	Catalytically Increased Prebiotic Peptide Formation: Ditryptophan, Dilysine, and Diserine. Origins of Life and Evolution of Biospheres, 2005, 35, 411-419.	1.9	26
116	Be(ii) in aqueous solutionâ€”an extended ab initio QM/MM MD study. Physical Chemistry Chemical Physics, 2006, 8, 2841-2847.	2.8	26
117	A quantum chemical analysis of the structural entities in aqueous sodium chloride solution and their concentration dependence.. Analytical Sciences, 1985, 1, 29-32.	1.6	25
118	Hydration of trivalent lanthanum revisited â€“ An ab initio QMCF-MD approach. Chemical Physics Letters, 2012, 536, 50-54.	2.6	25
119	Dynamics of ligand exchange mechanism at Cu(II) in water: An ab initio quantum mechanical charge field molecular dynamics study with extended quantum mechanical region. Journal of Chemical Physics, 2013, 139, 014503.	3.0	25
120	Application of multivariate data analysis methods to comparative molecular field analysis (CoMFA) data: proton affinities and pKa prediction for nucleic acids components. Journal of Computer-Aided Molecular Design, 1999, 13, 611-623.	2.9	24
121	Comparative docking studies on ligand binding to the multispecific antibodies IgE-La2 and IgE-Lb4. Journal of Computer-Aided Molecular Design, 1996, 10, 305-320.	2.9	23
122	QM/MMâ€“MD simulation of hydrated vanadium(II) ion. Chemical Physics Letters, 2002, 363, 367-371.	2.6	23
123	The influence of quantum forces on molecular dynamics simulation results for hydrated aluminium(III). Chemical Physics Letters, 2006, 422, 492-495.	2.6	23
124	The catalytic effect of l- and d-histidine on alanine and lysine peptide formation. Journal of Inorganic Biochemistry, 2008, 102, 2097-2102.	3.5	23
125	An ab initio quantum mechanical charge field molecular dynamics simulation of hydrogen peroxide in water. Computational and Theoretical Chemistry, 2012, 980, 15-22.	2.5	23
126	A Monte Carlo simulation of a supersaturated sodium chloride solution. Chemical Physics Letters, 1989, 155, 527-532.	2.6	22

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127	Classical and QM/MM molecular dynamics simulations of Co2+ in water. Chemical Physics, 2003, 295, 63-70.	1.9	22
128	The influence of heteroligands on the reactivity of Ni2+ in solution. Physical Chemistry Chemical Physics, 2005, 7, 1669.	2.8	22
129	Structure and dynamics of the [Zn(NH3)(H2O)5]2+ complex in aqueous solution obtained by an ab initio QM/MM molecular dynamics study. Physical Chemistry Chemical Physics, 2006, 8, 1675.	2.8	22
130	Quantum mechanical charge field molecular dynamics simulation of the TiO2+ ion in aqueous solution. Journal of Computational Chemistry, 2007, 28, 1704-1710.	3.3	22
131	A QMCF-MD Investigation of the Structure and Dynamics of Ce⁴⁺ in Aqueous Solution. Inorganic Chemistry, 2012, 51, 6746-6752.	4.0	22
132	Monte Carlo simulation of the peptide condensing system 0.5 M cupric chloride/5 M sodium chloride/water. The Journal of Physical Chemistry, 1992, 96, 4170-4174.	2.9	21
133	Structural and dynamical properties of Co(III) in aqueous solution: Ab initio quantum mechanical/molecular mechanical molecular dynamics simulation. Journal of Chemical Physics, 2003, 119, 6068-6072.	3.0	21
134	Stability of Different Zinc(II)â^'Diamine Complexes in Aqueous Solution with Respect to Structure and Dynamics:Â A QM/MM MD Study. Journal of Physical Chemistry B, 2007, 111, 151-158.	2.6	21
135	Influence of small cations on the rotational barrier of amides. Comparison of experiment with HCF-SCF model calculations. Journal of the Chemical Society, Faraday Transactions 2, 1975, 71, 1958.	1.1	20
136	Influence of alkali- and alkaline-earth-metal cations on the â€˜salt-induced peptide formationâ€™ reaction. Journal of the Chemical Society Dalton Transactions, 1994, , 1125-1130.	1.1	20
137	Catalytic effects of glycine on prebiotic divaline and diproline formation. Peptides, 2005, 26, 1109-1112.	2.4	20
138	The Hydration Structure of Sn(II): An ab initio Quantum Mechanical Charge Field Molecular Dynamics Study. Journal of Physical Chemistry B, 2009, 113, 4372-4378.	2.6	20
139	Structure and dynamics of hydrated <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si5.gif" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mi mathvariant="normal">Ag</mml:mi></mml:mrow><mml:mrow><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:mrow></mml: An ab initio quantum mechanical/charge field simulation. Chemical Physics Letters, 2010, 500, 251-255.	2.6	20
140	Structure and dynamics of the UO+2 ion in aqueous solution: an ab initio QMCF-MD study. Physical Chemistry Chemical Physics, 2010, 12, 11736.	2.8	20
141	Hydrogen bond formation of formamide and N-methylformamide in aqueous solution studied by quantum mechanical charge field-molecular dynamics (QMCF-MD). Physical Chemistry Chemical Physics, 2011, 13, 12173.	2.8	20
142	The Stability of Bisulfite and Sulfonate Ions in Aqueous Solution Characterized by Hydration Structure and Dynamics. Journal of Physical Chemistry B, 2012, 116, 11498-11507.	2.6	20
143	MESQUAC: mixed electrostaticâ€“quantum chemical approach to the description of large complexes. Journal of the Chemical Society, Faraday Transactions 2, 1979, 75, 178-183.	1.1	19
144	Comparative Molecular Field Analysis of Haptens Docked to the Multispecific Antibody IgE(Lb4). Journal of Medicinal Chemistry, 1996, 39, 3882-3888.	6.4	19

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145	Many-Body Effects in Combined Quantum Mechanical/Molecular Mechanical Simulations of the Hydrated Manganous Ion. Journal of Physical Chemistry A, 2002, 106, 9529-9532.	2.5	19
146	Ab Initio quantum mechanical charge field study of hydrated bicarbonate ion: Structural and dynamical properties. Journal of Computational Chemistry, 2010, 31, 249-257.	3.3	19
147	A Monte Carlo study on preferential solvation of lithium (I) in aqueous ammonia. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 643.	1.1	18
148	Structure of aqueous copper chloride solutions: results from Monte Carlo simulations at various concentrations. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 417.	1.7	18
149	Cu+in Liquid Ammonia and in Water:Â Intermolecular Potential Function and Monte Carlo Simulation. Journal of Physical Chemistry A, 1999, 103, 11115-11120.	2.5	18
150	The influence of small monovalent cations on neighbouring Nâ€¦Hî—¸O hydrogen bonds. Chemical Physics Letters, 1982, 88, 337-341.	2.6	17
151	Monte Carlo simulation of an 18.45 mol% aqueous ammonia solution. Journal of the Chemical Society, Faraday Transactions 2, 1988, 84, 679.	1.1	17
152	The influence of the Jahnâ€“Teller effect and of heteroligands on the reactivity of Cu2+. Chemical Communications, 2003, , 1286-1287.	4.1	17
153	Ag(I) ion in liquid ammonia. Chemical Physics Letters, 2004, 388, 395-399.	2.6	17
154	Ab Initio QM/MM Simulation of Ag+in 18.6% Aqueous Ammonia Solution:Â Structure and Dynamics Investigations. Journal of Physical Chemistry A, 2005, 109, 4437-4441.	2.5	17
155	A QM/MM MD simulation study of hydrated Pd2+. Chemical Physics Letters, 2006, 426, 301-305.	2.6	17
156	Tl(I)-the strongest structure-breaking metal ion in water? A quantum mechanical/molecular mechanical simulation study. Journal of Computational Chemistry, 2007, 28, 1006-1016.	3.3	17
157	The hydration of the mercury(I)-dimer â€“ A quantum mechanical charge field molecular dynamics study. Chemical Physics, 2008, 349, 210-218.	1.9	17
158	Guanidinium in aqueous solution studied by quantum mechanical charge field-molecular dynamics (QMCF-MD). Physical Chemistry Chemical Physics, 2012, 14, 7012.	2.8	17
159	Hydration of Mg2+ and its influence on the water hydrogen bonding network via ab initio QMCF MD. Chemical Physics Letters, 2012, 536, 39-44.	2.6	17
160	Combined Ab Initio Computational and Infrared Spectroscopic Study of the cis- and trans-Bis(glycinato)copper(II) Complexes in Aqueous Environment. Journal of Physical Chemistry Letters, 2013, 4, 1502-1506.	4.6	17
161	Solvent structures around Na+ and Cl? ions in water. Monatshefte FÃ¼r Chemie, 1985, 116, 1377-1383.	1.8	16
162	Molecular dynamics simulations of Na+ and Clâ˜ ions solvation in aqueous mixtures of formamide. Chemical Physics, 1997, 222, 43-57.	1.9	16

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163	Monte Carlo simulations of copper chloride solutions at various concentrations including full 3-body correction terms. Chemical Physics, 1997, 222, 281-288.	1.9	16
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