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	The properties of trivalent praseodymium, neodymium, promethium and samarium ions in water: A quantum mechanical molecular dynamics study. Chemical Physics Letters, 2015, 642, 12-16.	2.6	3
2	The lanthanoid hydration properties beyond the â€˜Gadolinium Breakâ€™: Dysprosium (III) and holmium (III), an ab initio quantum mechanical molecular dynamics study. Chemical Physics Letters, 2015, 635, 120-126.	2.6	11
3	The hydration properties of Gd(III) and Tb(III): An ab initio quantum mechanical molecular dynamics study. Chemical Physics Letters, 2015, 625, 116-120.	2.6	8
4	Thulium(III) and ytterbium(III) in aqueous solution ab initio quantum mechanical charge field molecular dynamics studies. Chemical Physics Letters, 2015, 638, 128-132.	2.6	5
5	Is the Hexacyanoferrate(II) Anion Stable in Aqueous Solution? A Combined Theoretical and Experimental Study. Inorganic Chemistry, 2015, 54, 10335-10341.	4.0	14
6	The hydration properties of Eu(II) and Eu(III): An ab initio quantum mechanical molecular dynamics study. Chemical Physics Letters, 2015, 618, 78-82.	2.6	13
7	Largely Reduced Grid Densities in a Vibrational Self-Consistent Field Treatment Do Not Significantly Impact the ResultingWavenumbers. Molecules, 2014, 19, 21253-21275.	3.8	12
8	Ionized <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si96.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CO</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml: and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si97.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SO</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:m in aqueous environment: Ab initio QM. Computational and Theoretical Chemistry, 2014, 1034, 85-93.	2.5	3
9	Ab initio quantum mechanical simulations confirm the formation of all postulated species in ionic dissociation. Physical Chemistry Chemical Physics, 2014, 16, 7368.	2.8	5
10	Structure and Dynamics of Chromatographically Relevant Fe(III)-Chelates. Journal of Physical Chemistry B, 2014, 118, 12232-12238.	2.6	4
11	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
12	Structure and dynamics of the Th4+-ion in aqueous solution â€“ An ab initio QMCF-MD study. Computational and Theoretical Chemistry, 2013, 1022, 94-102.	2.5	16
13	Erbium(III) in Aqueous Solution: An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry B, 2013, 117, 15151-15156.	2.6	11
14	Selective enrichment of phosphopeptides by a metalâ€“organic framework. Analytical Methods, 2013, 5, 2379.	2.7	36
15	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
16	A new type of metal chelate affinity chromatography using trivalent lanthanide ions for phosphopeptide enrichment. Analyst, The, 2013, 138, 2995.	3.5	43
17	Prebiotic Peptides. , 2013, , 1899-1903.		0
18	A QMCF-MD Investigation of the Structure and Dynamics of Ce⁴⁺ in Aqueous Solution. Inorganic Chemistry, 2012, 51, 6746-6752.	4.0	22

#	Article	IF	Citations
19	Characterization of structure and dynamics of an aqueous scandium(iii) ion by an extended ab initio QM/MM molecular dynamics simulation. Dalton Transactions, 2012, 41, 11889.	3.3	14
20	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
21	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
22	Computational study of the cerium(III) ion in aqueous environment. Chemical Physics Letters, 2012, 539-540, 50-53.	2.6	13
23	Simulation of Ir(III) in Aqueous Solution: The Most Inert Ion Hydrate. Australian Journal of Chemistry, 2012, 65, 1582.	0.9	7
24	Guanidinium in aqueous solution studied by quantum mechanical charge field-molecular dynamics (QMCF-MD). Physical Chemistry Chemical Physics, 2012, 14, 7012.	2.8	17
25	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
26	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
27	Chemical evolution from simple inorganic compounds to chiral peptides. Chemical Society Reviews, 2012, 41, 5484.	38.1	44
28	Simulation of electronic excitation in the liquid state by quantum mechanical charge field molecular dynamics. Chemical Physics Letters, 2012, 521, 74-77.	2.6	5
29	Hydration of trivalent lanthanum revisited â€“ An ab initio QMCF-MD approach. Chemical Physics Letters, 2012, 536, 50-54.	2.6	25
30	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
31	Structure and dynamics of the Zr⁴⁺ion in water. Physical Chemistry Chemical Physics, 2011, 13, 224-229.	2.8	29
32	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
33	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
34	Salt-Induced Peptide Formation in Chemical Evolution: Building Blocks Before RNA â€“ Potential of Peptide Splicing Reactions. , 2011, , 109-127.		2
35	Sulfur Dioxide in Water: Structure and Dynamics Studied by an Ab Initio Quantum Mechanical Charge Field Molecular Dynamics Simulation. Inorganic Chemistry, 2011, 50, 3379-3386.	4.0	15
36	Hydration of highly charged ions. Chemical Physics Letters, 2011, 512, 139-145.	2.6	48

#	Article	IF	Citations
37	Carbon dioxide in aqueous environmentâ€"A quantum mechanical charge field molecular dynamics study. International Journal of Quantum Chemistry, 2011, 111, 1370-1378.	2.0	13
38	Structure and dynamics of methanol in water: A quantum mechanical charge field molecular dynamics study. Journal of Computational Chemistry, 2011, 32, 886-892.	3.3	11
39	Computational study of the hafnium (IV) ion in aqueous solution. Chemical Physics Letters, 2011, 501, 292-295.	2.6	15
40	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
41	Hydrated germanium (II): Irregular structural and dynamical properties revealed by a quantum mechanical charge field molecular dynamics study. Journal of Computational Chemistry, 2010, 31, 278-285.	3.3	6
42	Temperature dependence of structure and dynamics of the hydrated Ca²⁺ ion according to ab initio quantum mechanical charge field and classical molecular dynamics. Journal of Computational Chemistry, 2010, 31, 1195-1200.	3.3	7
43	An ab initio quantum mechanical charge field molecular dynamics simulation of a dilute aqueous HCl solution. Journal of Computational Chemistry, 2010, 31, 1785-1792.	3.3	6
44	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
45	Arginine in the salt-induced peptide formation reaction: enantioselectivity facilitated by glycine, l- and d-histidine. Amino Acids, 2010, 39, 579-585.	2.7	7
46	The influence of the lone electron pair on structure and dynamics of divalent group IV metal ion hydrates. Journal of Molecular Liquids, 2010, 157, 79-82.	4.9	2
47	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></m An ab initio quantum mechanical/charge field simulation. Chemical Physics Letters, 2010, 500, 251-255.	2.6	20
48	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
49	Simulations of Liquids and Solutions Based on Quantum Mechanical Forces. Advances in Inorganic Chemistry, 2010, 62, 143-175.	1.0	56
50	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
51	Structural and Dynamic Aspects of Hydration of HAsO₄^{â"2}: An ab initio QMCF MD Simulation. Journal of Physical Chemistry B, 2010, 114, 3921-3926.	2.6	12
52	Structural and Dynamical Aspects of the Unsymmetric Hydration of Sb(III): An ab initio Quantum Mechanical Charge Field Molecular Dynamics Simulation. Inorganic Chemistry, 2010, 49, 2132-2140.	4.0	7
53	Determination of Structure and Dynamics of the Solvated Bisulfide (HS^{â"}) Ion by ab Initio QMCF Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 12883-12887.	2.6	11
54	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

#	Article	IF	Citations
55	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
56	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
57	Hydrolytic conversion of AsOâˆ'34 to HAsOâˆ'24: a QMCF MD study. Physical Chemistry Chemical Physics, 2010, 12, 6244.	2.8	4
58	Hydrolysis of tetravalent group IV metal ions: an ab initio simulation study. Physical Chemistry Chemical Physics, 2010, 12, 12423.	2.8	10
59	Structure and Dynamics of the Chromate Ion in Aqueous Solution. An ab Initio QMCF-MD Simulation. Inorganic Chemistry, 2010, 49, 7964-7968.	4.0	16
60	Inter- and intra-molecular OH stretching modes of bicarbonate in aqueous solution. Computational and Theoretical Chemistry, 2009, 913, 236-239.	1.5	9
61	Germanium(II) in water: An unusual hydration structure results of a QMCF MD simulation. Chemical Physics Letters, 2009, 470, 85-89.	2.6	13
62	Hydrolysis of As(III): A femtosecond process. Chemical Physics Letters, 2009, 473, 176-178.	2.6	16
63	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
64	Revisiting the Hydration of Pb(II): A QMCF MD Approach. Journal of Physical Chemistry B, 2009, 113, 13007-13013.	2.6	38
65	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
66	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
67	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
68	The hydrated platinum(ii) ion in aqueous solutionâ€"a combined theoretical and EXAFS spectroscopic study. Dalton Transactions, 2009, , 1512.	3.3	34
69	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
70	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
71	Methionine peptide formation under primordial earth conditions. Journal of Inorganic Biochemistry, 2008, 102, 1212-1217.	3.5	14
72	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

#	Article	IF	Citations
73	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
74	Quantum mechanical simulation studies of molecular vibrations and dynamics of oxo-anions in water. Chemical Physics, 2008, 346, 182-185.	1.9	36
75	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
76	Local density corrected three-body distribution functions for probing local structure reorganization in liquids. Physical Chemistry Chemical Physics, 2008, 10, 6653.	2.8	36
77	Structural and Dynamical Properties of Hydrogen Fluoride in Aqueous Solution: An ab Initio Quantum Mechanical Charge Field Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 12032-12037.	2.6	10
78	Exploring Structure and Dynamics of the Diaquotriamminezinc(II) Complex by QM/MM MD Simulation. Journal of Physical Chemistry B, 2008, 112, 5788-5794.	2.6	10
79	Molecular Dynamics Simulation Methods including Quantum Effects. Challenges and Advances in Computational Chemistry and Physics, 2008, , 247-278.	0.6	9
80	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
81	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
82	Computational Challenges in Simulation Methods for Liquids and Solutions. AIP Conference Proceedings, 2007, , .	0.4	1
83	Preferential Solvation and Dynamics of Ions Solvated in Mixed Solvents: Insights from QMâ^•MM MD Simulation Approach. AIP Conference Proceedings, 2007, , .	0.4	1
84	The First Steps of Chemical Evolution towards the Origin of Life. Chemistry and Biodiversity, 2007, 4, 2674-2702.	2.1	47
85	Quantum mechanical/molecular mechanical simulations of the Tl(III) ion in water. Journal of Computational Chemistry, 2007, 28, 1057-1067.	3.3	9
86	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
87	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
88	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
89	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
90	Be(ii) in aqueous solutionâ€"an extended ab initio QM/MM MD study. Physical Chemistry Chemical Physics, 2006, 8, 2841-2847.	2.8	26

#	Article	IF	Citations
91	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
92	Temperature Effects on the Structural and Dynamical Properties of the Zn(II)â˜Water Complex in Aqueous Solution:Â A QM/MM Molecular Dynamics Study. Journal of Physical Chemistry B, 2006, 110, 616-621.	2.6	12
93	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
94	The dynamics of the solvation of Pb(II) in aqueous solution obtained by an ab initio QM/MM MD approach. Chemical Physics, 2006, 323, 473-478.	1.9	9
95	The influence of quantum forces on molecular dynamics simulation results for hydrated aluminium(III). Chemical Physics Letters, 2006, 422, 492-495.	2.6	23
96	A QM/MM MD simulation study of hydrated Pd2+. Chemical Physics Letters, 2006, 426, 301-305.	2.6	17
97	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
98	Selective adsorption and reactivity of dipeptide stereoisomers in clay mineral suspension. Journal of Colloid and Interface Science, 2006, 294, 304-308.	9.4	12
99	Amino acids on the rampant primordial Earth: Electric discharges and the hot salty ocean. Molecular Diversity, 2006, 10, 3-7.	3.9	57
100	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
101	Prebiotic Peptides. , 2006, , 1481-1486.		3
102	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
103	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
104	Structural and dynamical properties of Bi3+ in water. Chemical Physics Letters, 2005, 406, 20-23.	2.6	16
105	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
106	Catalytically Increased Prebiotic Peptide Formation: Ditryptophan, Dilysine, and Diserine. Origins of Life and Evolution of Biospheres, 2005, 35, 411-419.	1.9	26
107	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
108	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

#	Article	IF	Citations
109	The influence of heteroligands on the reactivity of Ni2+ in solution. Physical Chemistry Chemical Physics, 2005, 7, 1669.	2.8	22
110	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
111	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
112	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
113	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
114	Catalytic effects of glycine on prebiotic divaline and diproline formation. Peptides, 2005, 26, 1109-1112.	2.4	20
115	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
116	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
117	Cuii in Liquid Ammonia: An Approach by Hybrid Quantum-Mechanical/Molecular-Mechanical Molecular Dynamics Simulation. ChemPhysChem, 2004, 5, 342-348.	2.1	26
118	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
119	Characterization of dynamics and reactivities of solvated ions byab initio simulations. Journal of Computational Chemistry, 2004, 25, 211-217.	3.3	261
120	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
121	Indications towards a stereoselectivity of the salt-induced peptide formation reaction. Inorganica Chimica Acta, 2004, 357, 649-656.	2.4	32
122	Structure and dynamics of hydrated ionsâ€”new insights through quantum mechanical simulations. Journal of Molecular Liquids, 2004, 110, 105-122.	4.9	94
123	Structure and dynamics of Co2+ in liquid ammonia: ab initio QM/MM molecular dynamics simulation. Chemical Physics, 2004, 305, 135-140.	1.9	7
124	Ag(I) ion in liquid ammonia. Chemical Physics Letters, 2004, 388, 395-399.	2.6	17
125	Influence of Electron Correlation Effects on the Solvation of Cu2+. Journal of the American Chemical Society, 2004, 126, 12786-12787.	13.7	49
126	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

#	Article	IF	Citations
127	â€œStructure Breakingâ€•Effect of Hydrated Cs+. Journal of Physical Chemistry A, 2004, 108, 1509-1514.	2.5	93
128	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
129	Gold(I) in Liquid Ammonia: Ab Initio QM/MM Molecular Dynamics Simulation. Journal of the American Chemical Society, 2004, 126, 9934-9935.	13.7	11
130	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
131	Many-body effects on structure and dynamics of aqueous ionic solutions. Journal of Computational Chemistry, 2003, 24, 1232-1239.	3.3	10
132	Classical and QM/MM molecular dynamics simulations of Co2+ in water. Chemical Physics, 2003, 295, 63-70.	1.9	22
133	Ultrafast ligand exchange rates determined by ab initio QM/MM molecular dynamics. Chemical Physics Letters, 2003, 382, 460-465.	2.6	11
134	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
135	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
136	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
137	MD and MC simulations of hydrated manganous ion including three-body effects. Computational and Theoretical Chemistry, 2003, 620, 15-20.	1.5	6
138	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
139	Molecular Docking Studies of Natural Cholinesterase-Inhibiting Steroidal Alkaloids fromSarcococcasaligna. Journal of Medicinal Chemistry, 2003, 46, 5087-5090.	6.4	42
140	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
141	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
142	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
143	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
144	The influence of the Jahnâ€“Teller effect and of heteroligands on the reactivity of Cu2+. Chemical Communications, 2003, , 1286-1287.	4.1	17

#	Article	IF	Citations
145	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
146	Molecular dynamics simulations of Hg2+ in aqueous solution includingN-body effects. Journal of Chemical Physics, 2003, 118, 5065-5070.	3.0	32
147	Extendedab initioquantum mechanical/molecular mechanical molecular dynamics simulations of hydrated Cu2+. Journal of Chemical Physics, 2003, 119, 9523-9531.	3.0	97
148	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
149	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
150	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
151	The hydration structure of the lithium ion. Journal of Chemical Physics, 2002, 117, 110-117.	3.0	133
152	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
153	QM/MMâ€“MD simulation of hydrated vanadium(II) ion. Chemical Physics Letters, 2002, 363, 367-371.	2.6	23
154	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
155	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
156	Classical and Mixed Quantum Mechanical/Molecular Mechanical Simulation of Hydrated Manganous Ion. Journal of Physical Chemistry A, 2001, 105, 7646-7650.	2.5	44
157	Preferential Cu2+ solvation in aqueous ammonia solution of various concentrations. Chemical Physics, 2001, 263, 1-6.	1.9	15
158	Calculation of sequence-dependent free energies of hydration of dipeptides formed by alanine and glycine. Journal of Computational Chemistry, 2001, 22, 846-860.	3.3	2
159	Dynamics of the solvation process of Ca2+ in water. Chemical Physics Letters, 2001, 349, 99-103.	2.6	49
160	Simulation of preferential Cu2+ solvation in aqueous ammonia solution by means of Monte Carlo method including three-body correction terms. Journal of Chemical Physics, 2000, 112, 4212-4215.	3.0	13
161	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
162	The effect of clay structure on peptide bond formation catalysis. Journal of Molecular Catalysis A, 1999, 144, 129-136.	4.8	52

#	Article	IF	Citations
163	Silica, alumina and clay catalyzed peptide bond formation: enhanced efficiency of alumina catalyst. , 1999, 29, 451-461.		81
164	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
165	Mutual amino acid catalysis in salt-induced peptide formation supports this mechanism's role in prebiotic peptide evolution. , 1999, 29, 463-471.		29
166	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
167	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
168	Are prions a relic of an early stage of peptide evolution?â˜†. Peptides, 1999, 20, 1513-1516.	2.4	27
169	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
170	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
171	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
172	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
173	Catalysis of dialanine formation by glycine in the salt-induced peptide formation reaction. , 1998, 28, 79-90.		36
174	Comparative molecular field analysis of artemisinin derivatives: ab initio versus semiempirical optimized structures. Journal of Computer-Aided Molecular Design, 1998, 12, 397-397.	2.9	14
175	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
176	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
177	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
178	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
179	Reaction-Path Dynamics of Hydroxyl Radical Reactions with Ethane and Haloethanes. Journal of Physical Chemistry A, 1997, 101, 4245-4253.	2.5	43
180	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

#	Article	IF	Citations
181	Solvated ion dynamics in the water-formamide mixtures using molecular dynamics simulations. Journal of Chemical Physics, 1997, 107, 6908-6916.	3.0	15
182	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
183	Molecular dynamics simulations of Na+ and Clâ" ions solvation in aqueous mixtures of formamide. Chemical Physics, 1997, 222, 43-57.	1.9	16
184	Glycine oligomerization on silica and alumina. Reaction Kinetics and Catalysis Letters, 1997, 62, 281-286.	0.6	46
185	Silica, Alumina, and Clay-Catalyzed Alanine Peptide Bond Formation. Journal of Molecular Evolution, 1997, 45, 457-466.	1.8	83
186	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
187	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
188	Comparative Molecular Field Analysis of Haptens Docked to the Multispecific Antibody IgE(Lb4). Journal of Medicinal Chemistry, 1996, 39, 3882-3888.	6.4	19
189	The effect of reaction conditions on montmorillonite-catalysed peptide formation. Catalysis Letters, 1996, 37, 267-272.	2.6	26
190	The effect of smectite composition on the catalysis of peptide bond formation. Journal of Molecular Evolution, 1996, 43, 326-333.	1.8	69
191	Investigation on the mechanism of peptide chain prolongation on montmorillonite. Journal of Inorganic Biochemistry, 1996, 61, 69-78.	3.5	34
192	A QM/MM simulation method applied to the solution of Li+ in liquid ammonia. Chemical Physics, 1996, 211, 313-323.	1.9	175
193	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
194	Preferential solvation study: Solvation of sodium chloride in water-hydroxylamine mixtures. Chemical Physics, 1996, 213, 77-93.	1.9	6
195	Monte Carlo Simulations of Zn(II) in Water Including Three-Body Effects. The Journal of Physical Chemistry, 1996, 100, 6808-6813.	2.9	54
196	The Effect of Smectite Composition on the Catalysis of Peptide Bond Formation. Journal of Molecular Evolution, 1996, 43, 326-333.	1.8	8
197	The Structure of Hydroxylamine â€" Water Mixtures. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1995, 50, 263-273.	1.5	5
198	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

#	Article	IF	Citations
199	Structure and dynamics of liquid formamide. Chemical Physics, 1995, 190, 61-82.	1.9	57
200	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
201	Application of Alternating Conditional Expectations Method to Quantitative Electronic Structure-Activity Relationships (QESAR). QSAR and Combinatorial Science, 1995, 14, 512-517.	1.2	1
202	Monte-Carlo Simulations of Cu(II) in Water with 3-Body Potential. The Journal of Physical Chemistry, 1995, 99, 15714-15717.	2.9	38
203	Solvation of lithium chloride in waterâ€“hydroxylamine mixtures: A theoretical investigation by means of Monte Carlo simulations. Journal of Chemical Physics, 1995, 102, 7602-7609.	3.0	11
204	Molecular dynamics simulations of aqueous formamide solution. II. Dynamics of solvent molecules. Journal of Chemical Physics, 1995, 102, 2920-2927.	3.0	33
205	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
206	Hydroxylamineâ€“water: intermolecular potential function and simulation of hydrated NH2OH. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 2337-2344.	1.7	10
207	Chloride Ion in Liquid Hydroxylamine: Pair Potential Function and Monte Carlo Simulation. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1994, 49, 797-801.	1.5	3
208	HPLC and electrochemical investigations of the salt-induced peptide formation from glycine, alanine, valine and aspartic acid under possible prebiotic conditions. Inorganica Chimica Acta, 1993, 207, 3-10.	2.4	15
209	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
210	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
211	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
212	Microstructure and species distribution of aqueous zinc chloride solutions: results from Monte Carlo simulations. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 1537.	1.7	12
213	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
214	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
215	Monte Carlo simulation of liquid hydroxylamine using ab initio intermolecular potential functions. International Journal of Quantum Chemistry, 1992, 42, 1339-1351.	2.0	4
216	Monte Carlo simulations of a magnesium ion in liquid ammonia. Chemical Physics, 1992, 162, 257-263.	1.9	9

#	Article	IF	Citations
217	Investigations on the mechanism of the salt-induced peptide formation. Origins of Life and Evolution of Biospheres, 1992, 22, 349-359.	1.9	37
218	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
219	Intermolecular Potential Function for Hydroxylamine Dimer Interactions from ab initio Calculations. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1991, 46, 32-38.	1.5	14
220	Monte Carlo Simulation of Magnesium Ion in 18.45 mol%Aqueous Ammonia Solution. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1991, 46, 111-116.	1.5	9
221	Salt-induced formation of mixed peptides under possible prebiotic conditions. Inorganica Chimica Acta, 1991, 186, 247-251.	2.4	45
222	Zinc ion in water: intermolecular potential with approximate three-body correction and Monte Carlo simulation. Chemical Physics, 1991, 156, 403-412.	1.9	35
223	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
224	A Monte Carlo simulation of a supersaturated sodium chloride solution. Chemical Physics Letters, 1989, 155, 527-532.	2.6	22
225	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
226	Quantum pharmacological analysis of structure-activity relationships for mefloquine antimalarial drugs.. Analytical Sciences, 1989, 5, 641-644.	1.6	9
227	Possible Role of Copper and Sodium Chloride in Prebiotic Evolution of Peptides. Analytical Sciences, 1989, 5, 411-414.	1.6	91
228	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
229	Simulation of preferential cation solvation in aqueous ammonia. Journal of the Chemical Society, Faraday Transactions 2, 1988, 84, 1779.	1.1	10
230	A Monte Carlo Study on a Magnesium Cyclen Complex. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1988, 43, 797-800.	1.5	0
231	Analysis of energetic effects in lithium fluoride crystals by means of ab-initio and MESQUAC-MO-SCF calculations.. Analytical Sciences, 1987, 3, 395-400.	1.6	0
232	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
233	Computational chemistry. A new tool for structural analysis.. Analytical Sciences, 1985, 1, 2-3.	1.6	0
234	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

#	Article	IF	Citations
235	Solvent structures around Na+ and Cl? ions in water. Monatshefte FÃ¼r Chemie, 1985, 116, 1377-1383.	1.8	16
236	Monte Carlo studies of the structure of NaCl aqueous solution at three different concentrations. Computational and Theoretical Chemistry, 1985, 121, 23-28.	1.5	12
237	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
238	The influence of small monovalent cations on neighbouring Nâ€¦Hî—¸O hydrogen bonds. Chemical Physics Letters, 1982, 88, 337-341.	2.6	17
239	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
240	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