Aqueous Solvation Free Energies of Ions and Ionâ^'Wate Value for the Absolute Aqueous Solvation Free Energy o

Journal of Physical Chemistry B

110, 16066-16081

DOI: 10.1021/jp063552y

Citation Report

#	Article	IF	Citations
19	Electronic tuning of Î²-diketiminate ligands with fluorinated substituents: effects on the O2-reactivity of mononuclear Cu(i) complexes. Dalton Transactions, 2006, , 4944-4953.	1.6	48
20	Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum. Journal of Chemical Physics, 2007, 126, 124114.	1.2	79
21	Self-Consistent Reaction Field Model for Aqueous and Nonaqueous Solutions Based on Accurate Polarized Partial Charges. Journal of Chemical Theory and Computation, 2007, 3, 2011-2033.	2.3	426
22	First-Principles Calculation of pK_a for Cocaine, Nicotine, Neurotransmitters, and Anilines in Aqueous Solution. Journal of Physical Chemistry B, 2007, 111, 10599-10605.	1.2	71
23	pKa Calculations of Aliphatic Amines, Diamines, and Aminoamides via Density Functional Theory with a Poissonâ"Boltzmann Continuum Solvent Model. Journal of Physical Chemistry A, 2007, 111, 4422-4430.	1.1	131
24	Hydration free energies of monovalent ions in transferable intermolecular potential four point fluctuating charge water: An assessment of simulation methodology and force field performance and transferability. Journal of Chemical Physics, 2007, 127, 064509.	1.2	107
25	Water-Assisted Hâ"H Bond Splitting Mediated by [CpRu(PTA)2Cl] (PTA=1,3,5-triaza-7-phosphaadamantane). A DFT Analysis. Organometallics, 2007, 26, 3289-3296.	1.1	57
26	Combined Quantum Mechanical and Molecular Mechanical Simulations of One- and Two-Electron Reduction Potentials of Flavin Cofactor in Water, Medium-Chain Acyl-CoA Dehydrogenase, and Cholesterol Oxidaseâ€. Journal of Physical Chemistry A, 2007, 111, 5729-5742.	1.1	73
27	Heterobimetallic Dioxygen Activation:Â Synthesis and Reactivity of Mixed Cuâ"Pd and Cuâ"Pt Bis(Î¼-oxo) Complexes. Journal of the American Chemical Society, 2007, 129, 7990-7999.	6.6	60
28	Single-Ion Solvation Free Energies and the Normal Hydrogen Electrode Potential in Methanol, Acetonitrile, and Dimethyl Sulfoxide. Journal of Physical Chemistry B, 2007, 111, 408-422.	1.2	452
29	Molecular Dynamics Simulations of Proteins:â€‰ Can the Explicit Water Model Be Varied?. Journal of Chemical Theory and Computation, 2007, 3, 1550-1560.	2.3	56
30	Computational Electrochemistry: The Aqueous Ru3+ | Ru2+Reduction Potential. Journal of Physical Chemistry C, 2007, 111, 5783-5799.	1.5	126
31	Can Electrophilicity Act as a Measure of the Redox Potential of Firstâ€Row Transition Metal Ions?. Chemistry - A European Journal, 2007, 13, 9331-9343.	1.7	55
32	On the Stereodivergent Behavior Observed in the Staudinger Reaction between Methoxyketene and (E)-N-Benzylidenearyl Amines. Angewandte Chemie - International Edition, 2007, 46, 3028-3032.	7.2	44
34	Accurate pKa determinations for some organic acids using an extended cluster method. Chemical Physics Letters, 2007, 439, 374-380.	1.2	37
35	Calculation of acidic dissociation constants in water: solvation free energy terms. Their accuracy and impact. Theoretical Chemistry Accounts, 2007, 118, 281-293.	0.5	69
36	Application of FT-ICR-MS for the study of proton-transfer reactions involving biomolecules. Analytical and Bioanalytical Chemistry, 2007, 389, 1365-1380.	1.9	22
37	Validation of density functional modeling protocols on experimental bis(Î¼-oxo)/Î¼-Î·2:Î·2-peroxo dicopper equilibria. Journal of Biological Inorganic Chemistry, 2007, 12, 1221-1234.	1.1	35

#	Article	IF	Citations
38	Dynamic polymer membranes displaying tunable transport properties on constitutional exchange. Journal of Membrane Science, 2008, 321, 8-14.	4.1	38
39	A new method of accurate pK_b determinations for some organic amines. International Journal of Quantum Chemistry, 2008, 108, 265-271.	1.0	3
40	Ionâ€Conduction Pathways in Selfâ€Organised Ureidoareneâ€“Heteropolysiloxane Hybrid Membranes. Chemistry - A European Journal, 2008, 14, 1776-1783.	1.7	46
41	Helicate Extension as a Route to Molecular Wires. Chemistry - A European Journal, 2008, 14, 7180-7185.	1.7	32
42	Alkali cation-Ï€ aromatic conduction pathways in self-organized hybrid membranes. Journal of Membrane Science, 2008, 321, 22-30.	4.1	26
43	Accurate calculation of the pKa of trifluoroacetic acid using high-level ab initio calculations. Chemical Physics Letters, 2008, 451, 163-168.	1.2	80
44	Determination of pKa for dithiophosphinic acids using density functional theory. Computational and Theoretical Chemistry, 2008, 867, 71-77.	1.5	22
45	Calculation of Solvation Free Energies of Charged Solutes Using Mixed Cluster/Continuum Models. Journal of Physical Chemistry B, 2008, 112, 9709-9719.	1.2	567
46	Hydration of Copper(II): New Insights from Density Functional Theory and the COSMO Solvation Model. Journal of Physical Chemistry A, 2008, 112, 9104-9112.	1.1	96
47	One-Electron and Two-Electron Transfers in Electrochemistry and Homogeneous Solution Reactions. Chemical Reviews, 2008, 108, 2113-2144.	23.0	324
48	Redox transitions of chromium, manganese, iron, cobalt and nickel protoporphyrins in aqueous solution. Physical Chemistry Chemical Physics, 2008, 10, 1023-1031.	1.3	62
49	The Ionic Work Function and its Role in Estimating Absolute Electrode Potentials. Langmuir, 2008, 24, 9868-9875.	1.6	168
50	A Universal Approach to Solvation Modeling. Accounts of Chemical Research, 2008, 41, 760-768.	7.6	536
51	Investigations of Acidity and Nucleophilicity of Diphenyldithiophosphinate Ligands Using Theory and Gas-Phase Dissociation Reactions. Inorganic Chemistry, 2008, 47, 3056-3064.	1.9	20
52	The Study of Redox Reactions on the Basis of Conceptual DFT Principles: EEM and Vertical Quantities. Journal of Physical Chemistry A, 2008, 112, 6023-6031.	1.1	53
53	Aqueous and Surface Redox Potentials from Self-Consistently Determined Gibbs Energies. Journal of Physical Chemistry C, 2008, 112, 8747-8750.	1.5	132
54	Acidâ€“base properties of a goethite surface model: A theoretical view. Geochimica Et Cosmochimica Acta, 2008, 72, 3587-3602.	1.6	50
55	Determination of Alkali and Halide Monovalent Ion Parameters for Use in Explicitly Solvated Biomolecular Simulations. Journal of Physical Chemistry B, 2008, 112, 9020-9041.	1.2	2,756

#	Article	IF	Citations
56	Theoretical Prediction of pK_a Values for Methacrylic Acid Oligomers Using Combined Quantum Mechanical and Continuum Solvation Methods. Journal of Physical Chemistry A, 2008, 112, 12687-12694.	1.1	59
57	Microhydration of Protonated Glycine:â€‰ An ab initio Family Tree. Journal of Physical Chemistry B, 2008, 112, 2430-2438.	1.2	42
58	Quantum Chemistry in Solution by Combining 3D Integral Equation Theory with a Cluster Embedding Approach. Journal of Physical Chemistry B, 2008, 112, 4337-4343.	1.2	69
59	Redox Transformations of Bis(2,2â€²-bipyridine)(1-methyl-1-pyridin-2-yl-ethylamine)ruthenium(II). Inorganic Chemistry, 2008, 47, 5314-5323.	1.9	5
60	Electronic structure calculations of liquid-solid interfaces: Combination of density functional theory and modified Poisson-Boltzmann theory. Physical Review B, 2008, 77, .	1.1	269
61	VBSM: A Solvation Model Based on Valence Bond Theory. Journal of Physical Chemistry A, 2008, 112, 12761-12768.	1.1	27
62	Charge-Dependent Cavity Radii for an Accurate Dielectric Continuum Model of Solvation with Emphasis on Ions: Aqueous Solutes with Oxo, Hydroxo, Amino, Methyl, Chloro, Bromo, and Fluoro Functionalities. Journal of Physical Chemistry A, 2008, 112, 10604-10613.	1.1	30
63	Ab initio molecular dynamics calculations of ion hydration free energies. Journal of Chemical Physics, 2009, 130, 204507.	1.2	111
64	Thermodynamically dominant hydration structures of aqueous ions. Journal of Chemical Physics, 2009, 130, 195102.	1.2	50
65	Directly Relating Gasâ€Phase Cluster Measurements to Solutionâ€Phase Hydrolysis, the Absolute Standard Hydrogen Electrode Potential, and the Absolute Proton Solvation Energy. Chemistry - A European Journal, 2009, 15, 5926-5934.	1.7	52
66	Î»â€Dynamics free energy simulation methods. Journal of Computational Chemistry, 2009, 30, 1692-1700.	1.5	164
67	Which functional groups of the molybdopterin ligand should be considered when modeling the active sites of the molybdenum and tungsten cofactors? A density functional theory study. Journal of Biological Inorganic Chemistry, 2009, 14, 1053-1064.	1.1	23
68	How accurate are continuum solvation models for drug-like molecules?. Journal of Computer-Aided Molecular Design, 2009, 23, 395-409.	1.3	68
69	Understanding the mechanism of the N-heterocyclic carbene-catalyzed ring-expansion of 4-formyl-Î²-lactams to succinimide derivatives. Tetrahedron, 2009, 65, 3432-3440.	1.0	59
70	Entropy contributions in pKa computation: Application to alkanolamines and piperazines. Computational and Theoretical Chemistry, 2009, 916, 1-9.	1.5	31
71	Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. Journal of Physical Chemistry B, 2009, 113, 6378-6396.	1.2	12,475
72	Computational Study of Copper(II) Complexation and Hydrolysis in Aqueous Solutions Using Mixed Cluster/Continuum Models. Journal of Physical Chemistry A, 2009, 113, 9559-9567.	1.1	110
73	Monoiron Hydrogenase Catalysis: Hydrogen Activation with the Formation of a Dihydrogen, Feâ€H^{Î´â€}Â·Â·Â·H^{Î´+}â€O, Bond and Methenyl-H₄MPT⁺ Triggered Hydride Transfer. Journal of the American Chemical Society, 2009, 131, 10901-10908.	6.6	158

#	Article	IF	Citations
74	Solvent Dependence of¹⁴N Nuclear Magnetic Resonance Chemical Shielding Constants as a Test of the Accuracy of the Computed Polarization of Solute Electron Densities by the Solvent. Journal of Chemical Theory and Computation, 2009, 5, 2284-2300.	2.3	9
75	Density Functional Study of Butadiyne to Butatrienylidene Isomerization in [Ru(HCâ‰¡CCâ‰¡CH)(PMe3)2(Cp)]+. Organometallics, 2009, 28, 6603-6616.	1.1	12
76	Spin Crossover-Coupled Electron Transfer of [M(tacn)2]3+/2+ Complexes (tacn =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 667 Td (1,4,7-T 6189-6197.	6.6	41
77	How Potentials of Zero Charge and Potentials for Water Oxidation to OH(ads) on Pt(111) Electrodes Vary With Coverage. Journal of Physical Chemistry C, 2009, 113, 17484-17492.	1.5	55
78	Accurate Benchmark Calculations on the Gas-Phase Basicities of Small Molecules. Journal of Physical Chemistry A, 2009, 113, 10096-10103.	1.1	18
79	Directly Relating Reduction Energies of Gaseous Eu(H₂O)_n³⁺, n = 55â^'140, to Aqueous Solution: The Absolute SHE Potential and Real Proton Solvation Energy. Journal of the American Chemical Society, 2009, 131, 13328-13337.	6.6	77
80	Theoretical Determination of the Redox Potentials of NRH:Quinone Oxidoreductase 2 Using Quantum Mechanical/Molecular Mechanical Simulations. Journal of Physical Chemistry B, 2009, 113, 8149-8157.	1.2	15
81	Complete Ion-Coordination Structure in the Rotor Ring of Na+-Dependent F-ATP Synthases. Journal of Molecular Biology, 2009, 391, 498-507.	2.0	98
82	Density functional theory for transition metals and transition metal chemistry. Physical Chemistry Chemical Physics, 2009, 11, 10757.	1.3	1,431
83	Absolute Hydration Entropies of Alkali Metal Ions from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 10255-10260.	1.2	41
84	The Ruâ^'Hbpp Water Oxidation Catalyst. Journal of the American Chemical Society, 2009, 131, 15176-15187.	6.6	253
85	Explicitly Representing the Solvation Shell in Continuum Solvent Calculations. Journal of Physical Chemistry A, 2009, 113, 6404-6409.	1.1	112
86	Rational design of ion force fields based on thermodynamic solvation properties. Journal of Chemical Physics, 2009, 130, 124507.	1.2	214
87	Anion Binding of Short, Flexible Aryl Triazole Oligomers. Journal of Organic Chemistry, 2009, 74, 8924-8934.	1.7	120
88	Redox potentials and pKa for benzoquinone from density functional theory based molecular dynamics. Journal of Chemical Physics, 2009, 131, 154504.	1.2	158
89	Universal Solvation Model Based on the Generalized Born Approximation with Asymmetric Descreening. Journal of Chemical Theory and Computation, 2009, 5, 2447-2464.	2.3	120
90	Parameterization and Validation of Solvation Corrected Atomic Radii. Journal of Physical Chemistry A, 2009, 113, 12028-12034.	1.1	16
91	Characterization of Redox States of Ru(OH₂)(Q)(tpy)²⁺ (Q =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 5 Experimental and Theoretical Studies. Inorganic Chemistry, 2009, 48, 4372-4383.	1.9	73

#	Article	IF	Citations
92	Estimation of the pKa values of water ligands in transition metal complexes using density functional theory with polarized continuum model solvent corrections. Dalton Transactions, 2009, , 10223.	1.6	55
93	Acidities of Water and Methanol in Aqueous Solution and DMSO. Journal of Chemical Education, 2009, 86, 864.	1.1	14
94	pK_a Calculation of Some Biologically Important Carbon Acids - An Assessment of Contemporary Theoretical Procedures. Journal of Chemical Theory and Computation, 2009, 5, 295-306.	2.3	131
95	Performance of SM6, SM8, and SMD on the SAMPL1 Test Set for the Prediction of Small-Molecule Solvation Free Energies. Journal of Physical Chemistry B, 2009, 113, 4538-4543.	1.2	418
96	Reply to Comment on â€œA Universal Approach to Solvation Modelingâ€• Accounts of Chemical Research, 2009, 42, 493-497.	7.6	69
97	Calculating solution redox free energies with ab initio quantum mechanical/molecular mechanical minimum free energy path method. Journal of Chemical Physics, 2009, 130, 164111.	1.2	35
98	Update of the CHARMM All-Atom Additive Force Field for Lipids: Validation on Six Lipid Types. Journal of Physical Chemistry B, 2010, 114, 7830-7843.	1.2	3,676
99	A theoretical study of the hydration of Rb+ by Monte Carlo simulations with refined ab initio-based model potentials. Theoretical Chemistry Accounts, 2010, 126, 197-211.	0.5	22
100	A universal approach for continuum solvent pK a calculations: are we there yet?. Theoretical Chemistry Accounts, 2010, 125, 3-21.	0.5	408
101	Theoretical pKa prediction of O-phosphoserine in aqueous solution. Chemical Physics Letters, 2010, 501, 123-129.	1.2	25
102	Platinum(II) complexes with thiourea derivatives containing oxygen, sulfur or selenium in a heterocyclic ring: computational studies and cytotoxic properties. Transition Metal Chemistry, 2010, 35, 639-647.	0.7	11
103	Thermodynamic stability of hydrogenâ€bonded systems in polar and nonpolar environments. Journal of Computational Chemistry, 2010, 31, 2046-2055.	1.5	24
105	A Unified pH Scale for All Phases. Angewandte Chemie - International Edition, 2010, 49, 6885-6888.	7.2	138
106	Iridium catalyzed hydrogenation of CO2 under basic conditionsâ€”Mechanistic insight from theoryâ˜†. Journal of Molecular Catalysis A, 2010, 324, 3-8.	4.8	101
107	A theoretical study on the efficient reversible redox-based switching of the second-order polarizabilities of two-dimensional nonlinear optical-active donorâ€“acceptor phenanthroline-hexamolybdate. Journal of Molecular Graphics and Modelling, 2010, 29, 13-20.	1.3	12
108	Theoretical study of the impact factor on redox property and second-order nonlinear response for organoimido derivatives of [Mo6O19]2â^': Electron donors with magnitude of conjugated groups or length of conjugated chain. Computational and Theoretical Chemistry, 2010, 947, 9-15.	1.5	2
109	Halide and sodium ion parameters for modeling aqueous solutions in TIP5P-Ew water. Chemical Physics Letters, 2010, 489, 113-117.	1.2	16
110	Theoretical studies on the pK~a~ values of perfluoroalkyl carboxylic acids. Nature Precedings, 0, , .	0.1	1

#	Article	IF	Citations
111	Theoretical investigation of electronic properties and redox properties for purely inorganic and aryloxide substituted Ti-containing POM derivatives. Molecular Physics, 2010, 108, 1553-1560.	0.8	3
112	Comment on â€œAb initio molecular dynamics calculation of ion hydration free energiesâ€•[J. Chem. Phys. 130, 204507 (2009)]. Journal of Chemical Physics, 2010, 133, 047103.	1.2	5
113	Comparative study on the gas to solution phase solvation free energies of model combustion flue gas compounds (N~2~, O~2~, CO~2~, H~2~O, SO~2~, and CO) in 178 organic solvents using the IEFPCM-UFF, CPCM, and SMD implicit solvent models at the Gaussian-4 (G4) level of theory. Nature Precedings, 2010, , .	0.1	1
114	Two-Electron Redox Energetics in Ligand-Bridged Dinuclear Molybdenum and Tungsten Complexes. Inorganic Chemistry, 2010, 49, 4611-4619.	1.9	24
115	Ligand Affinities Estimated by Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2010, 6, 1726-1737.	2.3	81
116	Using the Pyridine and Quinuclidine Scaffolds for Superbases: A DFT Study. Journal of Organic Chemistry, 2010, 75, 2651-2660.	1.7	35
117	Practically Efficient QM/MM Alchemical Free Energy Simulations: The Orthogonal Space Random Walk Strategy. Journal of Chemical Theory and Computation, 2010, 6, 2253-2266.	2.3	32
118	Dynamical Discrete/Continuum Linear Response Shells Theory of Solvation: Convergence Test for NH₄⁺ and OH^{â^’} Ions in Water Solution Using DFT and DFTB Methods. Journal of Physical Chemistry B, 2010, 114, 15941-15947.	1.2	20
119	Comparative DFT Analysis of Ligand and Solvent Effects on the Mechanism of H₂Activation in Water Mediated by Half-Sandwich Complexes [Cpâ€²Ru(PTA)₂Cl] (Cpâ€² =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 422 T Organometallics, 2010, 29, 5121-5131.	1.1	32
120	Astatine Standard Redox Potentials and Speciation in Acidic Medium. Journal of Physical Chemistry A, 2010, 114, 576-582.	1.1	65
121	Improved Density Functional Description of the Electrochemistry and Structureâ^’Property Descriptors of Substituted Flavins. Journal of Physical Chemistry B, 2010, 114, 14907-14915.	1.2	34
122	Cucurbituril Slippage: Translation is a Complex Motion. Organic Letters, 2010, 12, 2730-2733.	2.4	38
123	Microhydration of the Selenite Dianion: A Theoretical Study of Structures, Hydration Energies, and Electronic Stabilities of SeO₃^{2â^’}(H₂O)_n (n = 0â^’6, 9) Clusters. Journal of Physical Chemistry A, 2010, 114, 8948-8960.	1.1	8
124	Photocatalytic Water Oxidation at the GaN (101Ì…0)â^’Water Interface. Journal of Physical Chemistry C, 2010, 114, 13695-13704.	1.5	74
125	Influence of Explicit Hydration Waters in Calculating the Hydrolysis Constants for Geochemically Relevant Metals. Journal of Physical Chemistry A, 2010, 114, 1917-1925.	1.1	40
126	Accurate Estimates of Free Energy Changes in Charge Mutations. Journal of Chemical Theory and Computation, 2010, 6, 1884-1893.	2.3	16
127	Free Energies of Solvation with Surface, Volume, and Local Electrostatic Effects and Atomic Surface Tensions to Represent the First Solvation Shell. Journal of Chemical Theory and Computation, 2010, 6, 1109-1117.	2.3	53
128	First-Principles Prediction of the pK_as of Anti-inflammatory Oxicams. Journal of Physical Chemistry A, 2010, 114, 11992-12003.	1.1	44

#	Article	IF	Citations
129	Hosting anions. The energetic perspective. Chemical Society Reviews, 2010, 39, 3916.	18.7	119
130	Theoretical Calculations of Acid Dissociation Constants: A Review Article. Annual Reports in Computational Chemistry, 2010, , 113-138.	0.9	160
131	Molecular dynamics simulations of nonpolarizable inorganic salt solution interfaces: NaCl, NaBr, and NaI in transferable intermolecular potential 4-point with charge dependent polarizability (TIP4P-QDP) water. Journal of Chemical Physics, 2010, 132, 024713.	1.2	13
132	Accuracy of the microsolvationâ€“continuum approach in computing the pKa and the free energies of formation of phosphate species in aqueous solution. Physical Chemistry Chemical Physics, 2010, 12, 13804.	1.3	20
133	Counterion-dependent deuteration of pentamethylcyclopentadiene in water-soluble cationic Rh(iii) complexes assisted by PTA. Dalton Transactions, 2010, 39, 3366.	1.6	20
134	Dissolution Thermochemistry of Alkali Metal Dianion Salts (M₂X₁, M =) Tj ETQq1 1 0.784314 rgBT /Overloc	1.9	12
135	Metal-free catalysts for hydrogenation of both small and large imines: a computational experiment. Dalton Transactions, 2011, 40, 1929.	1.6	25
136	Reactivity of Aqueous Phase Hydroxyl Radical with Halogenated Carboxylate Anions: Experimental and Theoretical Studies. Environmental Science & Technology, 2011, 45, 6057-6065.	4.6	39
137	Computational Mechanistic Study on C_p*Ir Complex-Mediated Acceptorless Alcohol Dehydrogenation: Bifunctional Hydrogen Transfer vs Î²-H Elimination. Organometallics, 2011, 30, 2349-2363.	1.1	74
138	Electrostatic Polarization Is Crucial in Reproducing Cu(I) Interaction Energies and Hydration. Journal of Physical Chemistry B, 2011, 115, 10079-10085.	1.2	15
139	DFT and AIM Study of the Protonation of Nitrous Acid and the pK_aof Nitrous Acidium Ion. Journal of Physical Chemistry A, 2011, 115, 12357-12363.	1.1	18
140	Anion Adsorption and Adsorption/Desorption Kinetics onto/from Au(111) Electrodes Studied Using the Indirect Laser-Induced Temperature Jump Technique. Journal of Physical Chemistry C, 2011, 115, 2693-2704.	1.5	4
141	On the â€œReverse Gearâ€Mechanism of the Reversible Dehydrogenation/Hydrogenation of a Nitrogen Heterocycle Catalyzed by a C_p*Ir Complex: A Computational Study. Organometallics, 2011, 30, 3131-3141.	1.1	82
142	How Does the Nickel Pincer Complex Catalyze the Conversion of CO₂ to a Methanol Derivative? A Computational Mechanistic Study. Inorganic Chemistry, 2011, 50, 3816-3825.	1.9	159
143	Field-Extremum Model for Short-Range Contributions to Hydration Free Energy. Journal of Chemical Theory and Computation, 2011, 7, 3952-3960.	2.3	22
145	Reorganization Energy for Internal Electron Transfer in Multicopper Oxidases. Journal of Physical Chemistry B, 2011, 115, 13111-13126.	1.2	55
146	First-Principles-Based Multiscale, Multiparadigm Molecular Mechanics and Dynamics Methods for Describing Complex Chemical Processes. Topics in Current Chemistry, 2011, 307, 1-42.	4.0	9
147	Computation of methodology-independent single-ion solvation properties from molecular simulations. III. Correction terms for the solvation free energies, enthalpies, entropies, heat capacities, volumes, compressibilities, and expansivities of solvated ions. Journal of Chemical Physics, 2011, 134, 144103.	1.2	66

#	Article	IF	Citations
149	Water Oxidation by Mononuclear Ruthenium Complexes with TPA-Based Ligands. Inorganic Chemistry, 2011, 50, 10564-10571.	1.9	80
150	Electronic Structure of Oxidized Complexes Derived fromcis-[RuII(bpy)2(H2O)2]2+and Its Photoisomerization Mechanism. Inorganic Chemistry, 2011, 50, 11134-11142.	1.9	64
151	Proton Transfer between Tryptophan and Ionic Liquid Solvents Studied with Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 8231-8241.	1.2	22
152	On the impossibility of OH radical formation from the hydroxyl ion in water. Biophysics (Russian) Tj ETQq1 1 0.784314 rgBT /Overlock	0.2	3
153	Computational Study on the Catalytic Role of Pincer Ruthenium(II)-PNN Complex in Directly Synthesizing Amide from Alcohol and Amine: The Origin of Selectivity of Amide over Ester and Imine. Organometallics, 2011, 30, 5233-5247.	1.1	149
154	Modern methods for estimation of ionization constants of organic compounds in solution. Russian Journal of Organic Chemistry, 2011, 47, 1445-1467.	0.3	32
155	Redox Properties of Tanakaâ€™s Water Oxidation Catalyst: Redox Noninnocent Ligands Dominate the Electronic Structure and Reactivity. Inorganic Chemistry, 2011, 50, 5946-5957.	1.9	35
156	Firstâ€principles prediction of acidities in the gas and solution phase. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 649-660.	6.2	94
157	Insights into amine-based CO2 capture: an ab initio self-consistent reaction field investigation. Structural Chemistry, 2011, 22, 537-549.	1.0	21
158	Importance of iron as the metal ion in peptide deformylase: a biomimetic computational study. Theoretical Chemistry Accounts, 2011, 128, 137-146.	0.5	8
159	Avoiding gas-phase calculations in theoretical pK a predictions. Theoretical Chemistry Accounts, 2011, 130, 1-13.	0.5	65
160	Oxidation potential of thiophene oligomers: Theoretical and experimental approach. Journal of Polymer Science, Part B: Polymer Physics, 2011, 49, 1723-1733.	2.4	39
161	Reduction Potentials and Acidity Constants of Mn Superoxide Dismutase Calculated by QM/MM Freeâ€Energy Methods. ChemPhysChem, 2011, 12, 3337-3347.	1.0	38
162	Preferential Affinity of the Components of Liquid Mixtures at a Rigid Nonâ€Polar Surface: Enthalpic and Entropic Driving Forces. ChemPhysChem, 2011, 12, 3214-3223.	1.0	3
163	Anchor Points for the Unified BrÃ¸nsted Acidity Scale: The rCCC Model for the Calculation of Standard Gibbs Energies of Proton Solvation in Eleven Representative Liquid Media. Chemistry - A European Journal, 2011, 17, 5808-5826.	1.7	54
164	Theoretical insight into [Pd(en)(H2O)2]2+ binding to Guanine form [{Pd(en)(guanine)}4]4+: Kinetic control and thermodynamic control. Computational and Theoretical Chemistry, 2011, 967, 102-112.	1.1	1
165	Modeling short-range contributions to hydration energies with minimal parameterization. Chemical Physics Letters, 2011, 511, 161-165.	1.2	21
166	Electronic structure calculation study of metal complexes with a phytosiderophore mugineic acid. Inorganica Chimica Acta, 2011, 370, 304-310.	1.2	12

#	Article	IF	Citations
167	Calculating solvation energies by means of a fluctuating charge model combined with continuum solvent model. Journal of Chemical Physics, 2011, 134, 194115.	1.2	13
168	Computation of methodology-independent single-ion solvation properties from molecular simulations. IV. Optimized Lennard-Jones interaction parameter sets for the alkali and halide ions in water. Journal of Chemical Physics, 2011, 134, 144104.	1.2	136
169	Ion-water clusters, bulk medium effects, and ion hydration. Journal of Chemical Physics, 2011, 135, 054505.	1.2	19
170	Ions in Water and Biophysical Implications. , 2012, , .		40
171	Hybrid molecular dynamics and first-principles study on the work function of a Pt(111) electrode immersed in aqueous solution at room temperature. Physical Review B, 2012, 86, .	1.1	18
172	On the Effects of Changing Gaussian Program Version and SCRF Defining Parameters: Isopropylamine as a Case Study. Bulletin of the Chemical Society of Japan, 2012, 85, 962-975.	2.0	10
173	Thermodynamics and kinetics of CO2, CO, and H+ binding to the metal centre of CO2reductioncatalysts. Chemical Society Reviews, 2012, 41, 2036-2051.	18.7	632
174	New Interaction Parameters for Charged Amino Acid Side Chains in the GROMOS Force Field. Journal of Chemical Theory and Computation, 2012, 8, 3705-3723.	2.3	189
175	Structure of Charged Cyclohexyldiamines in Aqueous Solution: A Theoretical and Experimental Study. Journal of Physical Chemistry B, 2012, 116, 5019-5027.	1.2	6
176	Defined-sector explicit solvent in the continuum model approach for computational prediction of pK _a. Molecular Physics, 2012, 110, 2401-2412.	0.8	5
177	Self-assembly of ordered water tetramers in an encapsulated [Br(H2O)12]â^' complex. Chemical Communications, 2012, 48, 8631.	2.2	25
178	The Mechanism of Guanine Alkylation by Nitrogen Mustards: A Computational Study. Journal of Organic Chemistry, 2012, 77, 5914-5921.	1.7	74
179	CO2 capture in aqueous ammonia solutions: a computational chemistry perspective. Physical Chemistry Chemical Physics, 2012, 14, 16301.	1.3	15
180	A computational experiment to study hydrogenations of various unsaturated compounds catalyzed by a rationally designed metal-free catalyst. Dalton Transactions, 2012, 41, 4674.	1.6	19
181	Calculation of Derivative Thermodynamic Hydration and Aqueous Partial Molar Properties of Ions Based on Atomistic Simulations. Journal of Chemical Theory and Computation, 2012, 8, 3542-3564.	2.3	13
182	Computational Mechanistic Study of Câ€“C Coupling of Methanol and Allenes Catalyzed by an Iridium Complex. Organometallics, 2012, 31, 2066-2077.	1.1	5
183	Extension of Marcus Picture for Electron Transfer Reactions with Large Solvation Changes. Journal of the American Chemical Society, 2012, 134, 2067-2074.	6.6	42
184	Uranyl-Peroxide Nanocapsules: Electronic Structure and Cation Complexation in [(UO₂)₂₀(Î¼-O₂)₃₀]^{20â€“}. Inorganic Chemistry, 2012, 51, 3840-3845.	1.9	37

#	Article	IF	Citations
185	Thermochemical Parameters and pK_a Values for Chlorinated Congeners of Thiophenol. Journal of Chemical & Engineering Data, 2012, 57, 1834-1842.	1.0	14
186	Effects of Organic Solvent and Crystal Water on Î³-Chymotrypsin in Acetonitrile Media: Observations from Molecular Dynamics Simulation and DFT Calculation. Journal of Physical Chemistry B, 2012, 116, 3292-3304.	1.2	18
187	Quantum-Mechanical Study on the Aquaions and Hydrolyzed Species of Po(IV), Te(IV), and Bi(III) in Water. Journal of Physical Chemistry B, 2012, 116, 14903-14914.	1.2	7
188	Molecular Dynamics of Î²-Hairpin Models of Epigenetic Recognition Motifs. Journal of the American Chemical Society, 2012, 134, 15970-15978.	6.6	29
189	Intramolecular Interactions versus Hydration Effects on p-Guanidinoethyl-phenol Structure and pK_a Values. Journal of Physical Chemistry A, 2012, 116, 9404-9411.	1.1	14
190	Alignment of electronic energy levels at electrochemical interfaces. Physical Chemistry Chemical Physics, 2012, 14, 11245.	1.3	233
191	Quantum Chemical Benchmarking, Validation, and Prediction of Acidity Constants for Substituted Pyridinium Ions and Pyridinyl Radicals. Journal of Chemical Theory and Computation, 2012, 8, 3187-3206.	2.3	81
192	Improving the Capture of CO₂ by Substituted Monoethanolamines: Electronic Effects of Fluorine and Methyl Substituents. ChemPhysChem, 2012, 13, 3973-3980.	1.0	25
193	Computational Insight into the Mechanism of Selective Imine Formation from Alcohol and Amine Catalyzed by the Ruthenium(II)â€PNP Pincer Complex. European Journal of Inorganic Chemistry, 2012, 2012, 5011-5020.	1.0	79
195	Accurate pKa calculations for trimethylaminium ion with a variety of basis sets and methods combined with CPCM continuum solvation methods. Computational and Theoretical Chemistry, 2012, 999, 1-6.	1.1	11
196	Why the Mechanisms of Digermyne and Distannyne Reactions with H₂ Differ So Greatly. Journal of the American Chemical Society, 2012, 134, 8856-8868.	6.6	59
197	Quantum chemical characterization of the mechanism of a supported cobalt-based water oxidation catalyst. Dalton Transactions, 2012, 41, 12213.	1.6	58
198	Theoretical Determination of One-Electron Oxidation Potentials for Nucleic Acid Bases. Journal of Chemical Theory and Computation, 2012, 8, 5107-5123.	2.3	72
199	An accurate density functional theory based estimation of pKa values of polar residues combined with experimental data: from amino acids to minimal proteins. Physical Chemistry Chemical Physics, 2012, 14, 4181.	1.3	67
200	Pteridine-based fluorescent pH sensors designed for physiological applications. Journal of Photochemistry and Photobiology A: Chemistry, 2012, 247, 63-73.	2.0	14
201	Experimental and Computational Study of a New Wheel-Shaped {[W₅O₂₁]₃[(U^{VI}O₂)₂(Î¼-O₂)] Polyoxometalate. Inorganic Chemistry, 2012, 51, 8784-8790.	4.9	35
202	Ions. , 2012, , 49-98.		0
203	Charge Hydration Asymmetry: The Basic Principle and How to Use It to Test and Improve Water Models. Journal of Physical Chemistry B, 2012, 116, 9776-9783.	1.2	72

#	Article	IF	Citations
204	Molecular Modeling of the Reduction Mechanism in the Citrate-Mediated Synthesis of Gold Nanoparticles. Journal of Physical Chemistry C, 2012, 116, 23682-23691.	1.5	81
205	The aza-Moritaâ€“Baylisâ€“Hillman reaction of electronically and sterically deactivated substrates. Organic and Biomolecular Chemistry, 2012, 10, 3210.	1.5	19
207	Computational study of the proton affinity and basicity of structurally diverse Î±₁â€adrenoceptor ligands. Journal of Physical Organic Chemistry, 2012, 25, 351-360.	0.9	8
208	Computing redox potentials for dyes used in pâ€type dyeâ€sensitized solar cells. International Journal of Quantum Chemistry, 2012, 112, 3763-3768.	1.0	4
209	Reduction of Systematic Uncertainty in DFT Redox Potentials of Transition-Metal Complexes. Journal of Physical Chemistry C, 2012, 116, 6349-6356.	1.5	145
210	Automation of AMOEBA polarizable force field parameterization for small molecules. Theoretical Chemistry Accounts, 2012, 131, 1138.	0.5	134
211	Computational Mechanistic Study of the Hydrogenation of Carbonate to Methanol Catalyzed by the Ru^{II}PNN Complex. Inorganic Chemistry, 2012, 51, 5716-5727.	1.9	77
212	Quantum chemical characterization of the mechanism of an iron-based water oxidation catalyst. Chemical Science, 2012, 3, 1293.	3.7	122
213	Experimental and quantum chemical characterization of the water oxidation cycle catalysed by [RuII(damp)(bpy)(H2O)]2+. Chemical Science, 2012, 3, 2576.	3.7	96
214	A Self-Assembled Fluorideâ€“Water Cyclic Cluster of [F(H₂O)]₄^{4â€“} in a Molecular Box. Journal of the American Chemical Society, 2012, 134, 11892-11895.	6.6	43
215	Calculation of solvation free energies of Li+ and O2 â^' ions and neutral lithiumâ€“oxygen compounds in acetonitrile using mixed cluster/continuum models. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	41
216	Reaction Mechanism of Phosphaneâ€Catalyzed [4+2] Annulations between Î±â€Alkylallenoates and Activated Alkenes: A Computational Study. European Journal of Organic Chemistry, 2012, 2012, 3587-3597.	1.2	45
217	Importance of electrostatic polarizability in calculating cysteine acidity constants and copper(I) binding energy of Bacillus subtilis CopZ. Journal of Computational Chemistry, 2012, 33, 1142-1151.	1.5	15
218	The Kinetics and Thermodynamics of CO2Capture by Aqueous Ammonia Derived Using Meta-GGA Density Functional Theory and Wavefunction-Based Model Chemistry Methods. ACS Symposium Series, 2012, , 99-131.	0.5	1
219	Î²-Nitro-5,10,15-tritolylcorroles. Inorganic Chemistry, 2012, 51, 6928-6942.	1.9	54
220	The Reversible Opening of Water Channels in Cytochrome c Modulates the Heme Iron Reduction Potential. Journal of the American Chemical Society, 2012, 134, 13670-13678.	6.6	71
221	Bulk Gasâ€Phase Acidity. Chemistry - A European Journal, 2012, 18, 9333-9340.	1.7	16
222	Free energy partitioning analysis of the driving forces that determine ion density profiles near the water liquid-vapor interface. Journal of Chemical Physics, 2012, 136, 104503.	1.2	44

#	Article	IF	Citations
223	Improving the study of proton transfers between amino acid side chains in solution: choosing appropriate DFT functionals and avoiding hidden pitfalls. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	6
224	DFT/TDDFT investigation of the stepwise deprotonation in tetracycline: pKa assignment and UVâ€“vis spectroscopy. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	16
225	Reductive activation of the heme ironâ€“nitrosyl intermediate in the reaction mechanism of cytochrome c nitrite reductase: a theoretical study. Journal of Biological Inorganic Chemistry, 2012, 17, 741-760.	1.1	37
226	A reliable and efficient first principlesâ€based method for predicting pK_a values. III. Adding explicit water molecules: Can the theoretical slope be reproduced and pK_a values predicted more accurately?. Journal of Computational Chemistry, 2012, 33, 517-526.	1.5	54
227	Selective complexation of alkali metal ions using crown ethers derived from calix[4]arenes: a computational investigation of the structural and energetic factors. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2013, 75, 185-195.	1.6	2
228	Acidities of strong neutral BrÃ¸nsted acids in different media. Journal of Physical Organic Chemistry, 2013, 26, 162-170.	0.9	203
229	Why Mercury Prefers Soft Ligands. Journal of Physical Chemistry Letters, 2013, 4, 2317-2322.	2.1	54
230	Calculation of the Gibbs free energy of solvation and dissociation of HCl in water via Monte Carlo simulations and continuum solvation models. Physical Chemistry Chemical Physics, 2013, 15, 13578.	1.3	39
231	Fluorescent carboxylic and phosphonic acids: comparative photophysics from solution to organic nanoparticles. Physical Chemistry Chemical Physics, 2013, 15, 12748.	1.3	15
232	A Continuum Solvent Model of the Multipolar Dispersion Solvation Energy. Journal of Physical Chemistry B, 2013, 117, 9412-9420.	1.2	66
233	Computing pKa Values with a Mixing Hamiltonian Quantum Mechanical/Molecular Mechanical Approach. Journal of Chemical Theory and Computation, 2013, 9, 4257-4265.	2.3	11
234	Aggregation and Cooperative Effects in the Aldol Reactions of Lithium Enolates. Chemistry - A European Journal, 2013, 19, 13761-13773.	1.7	17
235	Development and application of effective pairwise potentials for UO2n+, NpO2n+, PuO2n+, and AmO2n+ (n = 1, 2) ions with water. Physical Chemistry Chemical Physics, 2013, 15, 15954.	1.3	42
236	Correspondence between Cluster-Ion and Bulk Solution Thermodynamic Properties: On the Validity of the Cluster-Pair-Based Approximation. Journal of Physical Chemistry A, 2013, 117, 11328-11338.	1.1	39
237	CHAPTER 1. Computational Modeling of Photocatalytic Cells. RSC Energy and Environment Series, 2013, , 1-36.	0.2	1
238	Fundamental insights into conformational stability and orbital interactions of antioxidant (+)-catechin species and complexation of (+)-catechin with zinc(II) and oxovanadium(IV). Journal of Molecular Structure, 2013, 1047, 344-357.	1.8	12
239	Thermochemical Factors Affecting the Dehalogenation of Aromatics. Environmental Science & Technology, 2013, 47, 14194-14203.	4.6	28
240	Bipolar switching polarity reversal by electrolyte layer sequence in electrochemical metallization cells with dual-layer solid electrolytes. Nanoscale, 2013, 5, 12598.	2.8	9

#	Article	IF	Citations
241	Predicting the stability of aprotic solvents in Li-air batteries: pKa calculations of aliphatic Câ€“H acids in dimethyl sulfoxide. Chemical Physics Letters, 2013, 558, 42-47.	1.2	49
242	A Polarizable Force Field of Dipalmitoylphosphatidylcholine Based on the Classical Drude Model for Molecular Dynamics Simulations of Lipids. Journal of Physical Chemistry B, 2013, 117, 9142-9160.	1.2	159
243	Generalized Born Solvation Model SM12. Journal of Chemical Theory and Computation, 2013, 9, 609-620.	2.3	170
244	Cluster-Continuum Calculations of Hydration Free Energies of Anions and Group 12 Divalent Cations. Journal of Chemical Theory and Computation, 2013, 9, 555-569.	2.3	44
245	The influence of water interfacial potentials on ion hydration in bulk water and near interfaces. Chemical Physics Letters, 2013, 561-562, 1-13.	1.2	102
246	Accurate pK_a Calculation of the Conjugate Acids of Alkanolamines, Alkaloids and Nucleotide Bases by Quantum Chemical Methods. ChemPhysChem, 2013, 14, 990-995.	1.0	25
247	Theoretical study on thermochemical parameters and pKa values for fluorinated isomers of toluene. Computational and Theoretical Chemistry, 2013, 1011, 21-29.	1.1	6
248	Torsional barriers of substituted biphenyls calculated using density functional theory: a benchmarking study. Organic and Biomolecular Chemistry, 2013, 11, 2859.	1.5	51
249	Defined-Sector Explicit Solvent in Continuum Cluster Model for Computational Prediction of pK_a: Consideration of Secondary Functionality and Higher Degree of Solvation. Journal of Chemical Theory and Computation, 2013, 9, 1027-1035.	2.3	10
250	Encapsulation of a discrete cyclic halide water tetramer [X2(H2O)2]2â^', X = Clâ^'/Brâ^' within a dimeric capsular assembly of a tripodal amide receptor. Chemical Communications, 2013, 49, 3997.	2.2	55
251	Direct Absolute pK_a Predictions and Proton Transfer Mechanisms of Small Molecules in Aqueous Solution by QM/MM-MD. Journal of Physical Chemistry B, 2013, 117, 6269-6275.	1.2	57
252	Inclusion complexes of Î²-cyclodextrine with organic ligands: molecular dynamics simulation of the thermodynamic stability in gas phase and in water solution. Molecular Simulation, 2013, 39, 442-452.	0.9	6
253	Mechanisms of Lactone Hydrolysis in Acidic Conditions. Journal of Organic Chemistry, 2013, 78, 6880-6889.	1.7	29
254	Mechanisms of Photoisomerization and Water-Oxidation Catalysis of Mononuclear Ruthenium(II) Monoaquo Complexes. Inorganic Chemistry, 2013, 52, 6354-6364.	1.9	67
255	A generalized any-particle propagator theory: Prediction of proton affinities and acidity properties with the proton propagator. Journal of Chemical Physics, 2013, 138, 194108.	1.2	28
256	Theoretical investigation of the alloxan-dialuric acid redox cycle. International Journal of Quantum Chemistry, 2013, 113, 2060-2069.	1.0	14
257	Toward the accurate calculation of pKa values in water and acetonitrile. Biochimica Et Biophysica Acta - Bioenergetics, 2013, 1827, 882-891.	0.5	112
258	A Density Functional Theory Based Protocol to Compute the Redox Potential of Transition Metal Complex with the Correction of Pseudo-Counterion: General Theory and Applications. Journal of Chemical Theory and Computation, 2013, 9, 2974-2980.	2.3	36

#	Article	IF	Citations
259	Explicit Solvation Shell Model and Continuum Solvation Models for Solvation Energy and pK_a Determination of Amino Acids. Journal of Chemical Theory and Computation, 2013, 9, 5021-5037.	2.3	42
260	Hydrogenation of Dimethyl Carbonate to Methanol by trans-[Ru(H)₂(PNN)(CO)] Catalysts: DFT Evidence for Ion-Pair-Mediated Metathesis Paths for Câ€“OMe Bond Cleavage. Organometallics, 2013, 32, 6969-6985.	1.1	49
261	Theoretical Study of the Protonation of the One-Electron-Reduced Guanineâ€“Cytosine Base Pair by Water. Journal of Physical Chemistry B, 2013, 117, 2096-2105.	1.2	14
262	A Continuum Model of Solvation Energies Including Electrostatic, Dispersion, and Cavity Contributions. Journal of Physical Chemistry B, 2013, 117, 9421-9429.	1.2	76
263	Stability of Flavin Semiquinones in the Gas Phase: The Electron Affinity, Proton Affinity, and Hydrogen Atom Affinity of Lumiflavin. Journal of Physical Chemistry A, 2013, 117, 11136-11141.	1.1	18
264	Computational Prediction of One-Electron Reduction Potentials and Acid Dissociation Constants for Guanine Oxidation Intermediates and Products. Journal of Physical Chemistry B, 2013, 117, 9518-9531.	1.2	43
265	Determination of New Cu⁺, Cu²⁺, and Zn²⁺ Lennard-Jones Ion Parameters in Acetonitrile. Journal of Physical Chemistry B, 2013, 117, 10513-10522.	1.2	20
266	Consistent scheme for computing standard hydrogen electrode and redox potentials. Journal of Computational Chemistry, 2013, 34, 21-26.	1.5	39
267	Metal-Salens As Catalysts In Electroreductive Cyclization and Electrohydrocyclization: Computational and Experimental Studies. Journal of the Electrochemical Society, 2013, 160, G3080-G3090.	1.3	5
268	p of silicic acid in presence of La³⁺using single sweep method coupled to DFT-based molecular dynamics. Molecular Physics, 2013, 111, 3478-3485.	0.8	1
270	Self-consistent continuum solvation (SCCS): The case of charged systems. Journal of Chemical Physics, 2013, 139, 214110.	1.2	90
271	Photophysical and ligand binding studies of metalloporphyrins bearing hydrophilic distal superstructure. Journal of Porphyrins and Phthalocyanines, 2013, 17, 210-219.	0.4	5
272	Ab initiocalculation of the deprotonation constants of an atomistically defined nanometer-sized, aluminium hydroxide oligomer. Molecular Simulation, 2013, 39, 220-227.	0.9	1
273	DFT Study on Thermodynamic Parameters of CO2 Absorption into Aqueous Solution of Aliphatic Amines. Chinese Journal of Chemical Physics, 2014, 27, 672-678.	0.6	3
274	The thermodynamics of proton hydration and the electrochemical surface potential of water. Journal of Chemical Physics, 2014, 141, 18C512.	1.2	36
275	Quasichemical analysis of the cluster-pair approximation for the thermodynamics of proton hydration. Journal of Chemical Physics, 2014, 140, 224507.	1.2	25
276	Simplified continuum solvent model with a smooth cavity based on volumetric data. Journal of Chemical Physics, 2014, 141, 174108.	1.2	58
277	A scaled-ionic-charge simulation model that reproduces enhanced and suppressed water diffusion in aqueous salt solutions. Journal of Chemical Physics, 2014, 141, 104507.	1.2	109

#	Article	IF	Citations
278	The Protoelectric Potential Map (PPM): An Absolute Twoâ€Dimensional Chemical Potential Scale for a Global Understanding of Chemistry. Chemistry - A European Journal, 2014, 20, 4194-4211.	1.7	42
279	A density functional theory study of complex species and reactions of Am(III)/Eu(III) with nitrate anions. Molecular Simulation, 2014, 40, 379-386.	0.9	17
280	Computational insight into Wilkinson's complex catalyzed [2Â+Â2Â+Â2] cycloaddition mechanism leading to pyridine formation. Journal of Organometallic Chemistry, 2014, 768, 15-22.	0.8	15
281	Computational Redox Potential Predictions: Applications to Inorganic and Organic Aqueous Complexes, and Complexes Adsorbed to Mineral Surfaces. Minerals (Basel, Switzerland), 2014, 4, 345-387.	0.8	56
282	High-level ab initio calculation of the stability of mercuryâ€“thiolate complexes. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	14
283	DFT-B3LYP and SMD study on the interactions between aza-, diaza-, and triaza-12-crown-4 (A n) Tj ETQq1 1 0.784314 rgBT /Overlock 10 25, 919-929.	1.0	10
284	Selective Catalytic Deuterium Labeling of Alcohols during a Transfer Hydrogenation Process of Ketones Using D2O as the Only Deuterium Source. Theoretical and Experimental Demonstration of a Ruâ€“H/D+Exchange as the Key Step. ACS Catalysis, 2014, 4, 1040-1053.	5.5	44
285	What Can Density Functional Theory Tell Us about Artificial Catalytic Water Splitting?. Inorganic Chemistry, 2014, 53, 6386-6397.	1.9	126
286	Phosphine-Substituted (Î·5-Pentadienyl) Manganese Carbonyl Complexes: Geometric Structures, Electronic Structures, and Energetic Properties of the Associative Substitution Mechanism, Including Isolation of the Slipped Î·3-Pentadienyl Associative Intermediate. Organometallics, 2014, 33, 278-288.	1.1	9
287	Calculations of One-Electron Redox Potentials of Oxoiron(IV) Porphyrin Complexes. Journal of Chemical Theory and Computation, 2014, 10, 243-251.	2.3	47
288	Absolute redox potential of liquid water: a first-principles theory. Chemical Science, 2014, 5, 1216-1220.	3.7	9
289	Dissociation Constants of Weak Acids from ab Initio Molecular Dynamics Using Metadynamics: Influence of the Inductive Effect and Hydrogen Bonding on pK_a Values. Journal of Physical Chemistry B, 2014, 118, 13651-13657.	1.2	51
290	Reduction potential predictions of some aromatic nitrogen-containing molecules. RSC Advances, 2014, 4, 57442-57451.	1.7	58
291	Comparison of the Active-Site Design of Molybdenum Oxo-Transfer Enzymes by Quantum Mechanical Calculations. Inorganic Chemistry, 2014, 53, 11913-11924.	1.9	17
292	One electron oxidation potential as a predictor of rate constants of N-containing compounds with carbonate radical and triplet excited state organic matter. Environmental Sciences: Processes and Impacts, 2014, 16, 832-838.	1.7	42
293	Electrochemical, spectroscopic and theoretical studies of a simple bifunctional cobalt corrole catalyst for oxygen evolution and hydrogen production. Physical Chemistry Chemical Physics, 2014, 16, 1883-1893.	1.3	188
294	Investigation of the Redox Chemistry of Anthraquinone Derivatives Using Density Functional Theory. Journal of Physical Chemistry A, 2014, 118, 8852-8860.	1.1	135
295	Computational electrochemistry: prediction of liquid-phase reduction potentials. Physical Chemistry Chemical Physics, 2014, 16, 15068-15106.	1.3	407

#	Article	IF	Citations
296	Rational design of Co-based redox mediators for dye-sensitized solar cells by density functional theory. RSC Advances, 2014, 4, 31544-31551.	1.7	24
297	A non-Bornian analysis of the Gibbs energy of hydration for organic ions. RSC Advances, 2014, 4, 27634-27641.	1.7	8
298	Simulated Solvation of Organic Ions: Protonated Methylamines in Water Nanodroplets. Convergence toward Bulk Properties and the Absolute Proton Solvation Enthalpy. Journal of Physical Chemistry B, 2014, 118, 6222-6233.	1.2	15
299	Assessing the performance of MM/PBSA and MM/GBSA methods. 4. Accuracies of MM/PBSA and MM/GBSA methodologies evaluated by various simulation protocols using PDBbind data set. Physical Chemistry Chemical Physics, 2014, 16, 16719-16729.	1.3	586
300	Theoretical Study of the Formation of Mercury (Hg²⁺) Complexes in Solution Using an Explicit Solvation Shell in Implicit Solvent Calculations. Journal of Physical Chemistry B, 2014, 118, 11271-11283.	1.2	16
301	Approach for Predicting the Standard Free Energy Solvation of H⁺ and Acidity Constant in Nonaqueous Organic Solvents. Journal of Chemical & Engineering Data, 2014, 59, 3555-3564.	1.0	12
302	Role of Acetate and Water in the Water-Assisted Pd(OAc)₂-Catalyzed Cross-Coupling of Alkenes with N-Tosyl Hydrazones: A DFT Study. Organometallics, 2014, 33, 3453-3463.	1.1	22
303	Mechanistic Insights into the Catalysis of Electrochemical Proton Reduction by a Diiron Azadithiolate Complex. Inorganic Chemistry, 2014, 53, 10667-10673.	1.9	42
305	Theoretical Studies on a New Class of Câ€“C Bond Formation: Palladium-Catalyzed Reactions of Î±-Diazocarbonyl Compounds with Allylic Esters. Organometallics, 2014, 33, 1404-1415.	1.1	25
306	Protonation/deprotonation process of Emodin in aqueous solution and pKa determination: UV/Visible spectrophotometric titration and quantum/molecular mechanics calculations. Chemical Physics, 2014, 440, 69-79.	0.9	39
307	New Water Oxidation Chemistry of a Seven-Coordinate Ruthenium Complex with a Tetradentate Polypyridyl Ligand. Inorganic Chemistry, 2014, 53, 6904-6913.	1.9	48
308	Is Nitrate Anion Photodissociation Mediated by Singletâ€“Triplet Absorption?. Journal of Physical Chemistry Letters, 2014, 5, 1958-1962.	2.1	15
309	Solv-ccCA: Implicit Solvation and the Correlation Consistent Composite Approach for the Determination of pK_a. Journal of Chemical Theory and Computation, 2014, 10, 1500-1510.	2.3	21
310	Electronic Effects on a Mononuclear Co Complex with a Pentadentate Ligand for Catalytic H₂ Evolution. Inorganic Chemistry, 2014, 53, 10094-10100.	1.9	79
311	Ion Interactions with the Airâ€“Water Interface Using a Continuum Solvent Model. Journal of Physical Chemistry B, 2014, 118, 8700-8710.	1.2	40
312	Strictly Conserved Lysine of Prolyl-tRNA Synthetase Editing Domain Facilitates Binding and Positioning of Misacylated tRNA^{Pro}. Biochemistry, 2014, 53, 1059-1068.	1.2	19
313	Force Field Independent Metal Parameters Using a Nonbonded Dummy Model. Journal of Physical Chemistry B, 2014, 118, 4351-4362.	1.2	148
314	Photoemission Spectra and Density Functional Theory Calculations of 3d Transition Metalâ€“Aqua Complexes (Tiâ€“Cu) in Aqueous Solution. Journal of Physical Chemistry B, 2014, 118, 6850-6863.	1.2	28

#	Article	IF	Citations
315	Development of Monopole Interaction Models for Ionic Compounds. Part I: Estimation of Aqueous Henryâ€™s Law Constants for Ions and Gas Phase pK_a Values for Acidic Compounds. Molecular Informatics, 2014, 33, 92-103.	1.4	1
316	Ice Crystallization in Ultrafine Waterâ€“Salt Aerosols: Nucleation, Ice-Solution Equilibrium, and Internal Structure. Journal of the American Chemical Society, 2014, 136, 8081-8093.	6.6	59
317	Solvation and Protonation of Coumarin 102 in Aqueous Media: A Fluorescence Spectroscopic and Theoretical Study. Journal of Physical Chemistry A, 2014, 118, 5238-5247.	1.1	15
318	Toward a Molecular Understanding of Energetics in Liâ€“S Batteries Using Nonaqueous Electrolytes: A High-Level Quantum Chemical Study. Journal of Physical Chemistry C, 2014, 118, 11545-11558.	1.5	154
319	DFT calculations on H, OH and O adsorbate formations on Pt(111) and Pt(332) electrodes. Journal of Electroanalytical Chemistry, 2014, 716, 31-44.	1.9	85
320	Polymer supported organic catalysts for O2 reduction in Li-O2 batteries. Electrochimica Acta, 2014, 119, 138-143.	2.6	18
321	A Non-Bornian Analysis of the Gibbs Energy of Ion Hydration. Bulletin of the Chemical Society of Japan, 2014, 87, 403-411.	2.0	8
322	Meaning and Measurability of Singleâ€ion Activities, the Thermodynamic Foundations of pH, and the Gibbs Free Energy for the Transfer of Ions between Dissimilar Materials. ChemPhysChem, 2015, 16, 1978-1991.	1.0	28
323	Techniques For Studies Of Electrochemical Reactions In Solution. , 2015, , 117-188.		10
324	A classical force field for tetrahedral oxyanions developed using hydration properties: The examples of pertechnetate (TcO4â^') and sulfate (SO42â^'). Journal of Chemical Physics, 2015, 143, 174502.	1.2	24
325	Preparation and characterization of thermoplastic waterâ€borne polycarbonateâ€based polyurethane dispersions and cast films. Journal of Applied Polymer Science, 2015, 132, .	1.3	21
326	Aqueous acidities of primary benzenesulfonamides: Quantum chemical predictions based on density functional theory and SMD. Journal of Computational Chemistry, 2015, 36, 2158-2167.	1.5	10
327	Mechanisms and Factors Controlling Photoisomerization Equilibria, Ligand Exchange, and Water Oxidation Catalysis Capabilities of Mononuclear RuthenÂium(II) Complexes. European Journal of Inorganic Chemistry, 2015, 2015, 3892-3903.	1.0	16
329	Photoinduced Water Oxidation at the Aqueous GaN (101Ì…0) Interface: Deprotonation Kinetics of the First Proton-Coupled Electron-Transfer Step. ACS Catalysis, 2015, 5, 2317-2323.	5.5	33
330	Accurate Evaluation of Charge Asymmetry in Aqueous Solvation. Journal of Physical Chemistry B, 2015, 119, 6092-6100.	1.2	16
331	Computational estimation of pK_a values. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 290-297.	6.2	85
332	On the Reaction Mechanism of the Rhodium-Catalyzed Arylation of Fullerene (C₆₀) with Organoboron Compounds in the Presence of Water. ChemistryOpen, 2015, 4, 774-778.	0.9	12
333	Refined Dummy Atom Model of Mg²⁺ by Simple Parameter Screening Strategy with Revised Experimental Solvation Free Energy. Journal of Chemical Information and Modeling, 2015, 55, 2575-2586.	2.5	26

#	Article	IF	Citations
334	Theoretical Analysis of the Oxidation Potentials of Organic Electrolyte Solvents. ECS Electrochemistry Letters, 2015, 4, A103-A105.	1.9	9
335	Inclusion compounds based on nickel(II) dimethylglyoxymate and cucurbit[8]uril: A quantum chemical prediction of the structure and thermodynamic parameters of formation. Journal of Structural Chemistry, 2015, 56, 1449-1457.	0.3	3
336	Inclusion compound based on Bis(ethylenediamine)copper(II) complex and cucurbit[8]uril: Quantum chemical prediction for structure and formation thermodynamic parameters. Russian Journal of Inorganic Chemistry, 2015, 60, 1247-1252.	0.3	7
337	Calculation of acidity/basicity values of some fluorinated compounds in gas phase and aqueous solution: A computational approach. Computational and Theoretical Chemistry, 2015, 1054, 71-79.	1.1	10
338	Theoretical investigation on the chemoselective N-heterocyclic carbene-catalyzed cross-benzoin reactions. Organic and Biomolecular Chemistry, 2015, 13, 3654-3661.	1.5	35
339	Accurate Standard Hydrogen Electrode Potential and Applications to the Redox Potentials of Vitamin C and NAD/NADH. Journal of Physical Chemistry A, 2015, 119, 369-376.	1.1	102
340	Estimating successive pK_a values of polyprotic acids from ab initio molecular dynamics using metadynamics: the dissociation of phthalic acid and its isomers. Physical Chemistry Chemical Physics, 2015, 17, 6383-6388.	1.3	37
341	Acidity of the Amidoxime Functional Group in Aqueous Solution: A Combined Experimental and Computational Study. Journal of Physical Chemistry B, 2015, 119, 3567-3576.	1.2	54
342	Unified pH Values of Liquid Chromatography Mobile Phases. Analytical Chemistry, 2015, 87, 2623-2630.	3.2	46
343	Thermodynamics of Small Alkali Metal Halide Cluster Ions: Comparison of Classical Molecular Simulations with Experiment and Quantum Chemistry. Journal of Physical Chemistry A, 2015, 119, 488-500.	1.1	7
344	Chemically and Electrochemically Triggered Assembly of Viologen Radicals: Towards Multiaddressable Molecular Switches. Chemistry - A European Journal, 2015, 21, 2090-2106.	1.7	32
345	Cluster Models for Studying CO2 Reduction on Semiconductor Photoelectrodes. Topics in Catalysis, 2015, 58, 46-56.	1.3	30
346	How a [Co^{IV}${^{underline{.....}}}$O]²⁺ Fragment Oxidizes Water: Involvement of a Biradicaloid [Co^{II}â€"(â‹…Oâ‹…)]²⁺ Species in Forming the Oï£¿O Bond. ChemSusChem, 2015, 8, 844-852.	3.6	46
347	Conceptual Quantum Chemical Analysis of Bonding and Noncovalent Interactions in the Formation of Frustrated Lewis Pairs. Chemistry - A European Journal, 2015, 21, 5510-5519.	1.7	30
348	Theoretical insights into the mechanism of redox switch in heat shock protein Hsp33. Journal of Biological Inorganic Chemistry, 2015, 20, 555-562.	1.1	15
349	Towards the Discrimination of Carboxylates by Hydrogenâ€Bond Donor Anion Receptors. Chemistry - A European Journal, 2015, 21, 5145-5160.	1.7	34
350	Hydronium and hydroxide at the airâ€"water interface with a continuum solvent model. Chemical Physics Letters, 2015, 635, 1-12.	1.2	44
351	Stability and spatial arrangement of the 2,4-dichlorophenoxyacetic acid and Î²-cyclodextrin inclusion compound: A theoretical study. Chemical Physics Letters, 2015, 633, 158-162.	1.2	10

#	Article	IF	Citations
352	Electrochemical Reduction of 2,4-Dinitrotoluene in Aprotic and pH-Buffered Media. Journal of Physical Chemistry C, 2015, 119, 13088-13097.	1.5	33
353	A theoretical investigation of substituent effects on the stability and reactivity of N-heterocyclic olefin carboxylates. Organic and Biomolecular Chemistry, 2015, 13, 8533-8544.	1.5	26
354	Accurate quantum chemical modelling of the separation of Eu³⁺from Am³⁺/Cm³⁺by liquidâ€“liquid extraction with Cyanex272. Physical Chemistry Chemical Physics, 2015, 17, 20605-20616.	1.3	41
355	Coextraction of Water into Nitrobenzene with Organic Ions. Journal of Physical Chemistry B, 2015, 119, 6010-6017.	1.2	9
356	Ab Initio Electrochemistry: Exploring the Hydrogen Evolution Reaction on Carbon Nanotubes. Journal of Physical Chemistry C, 2015, 119, 16166-16178.	1.5	45
357	Impacts of electrode potentials and solvents on the electroreduction of CO₂: a comparison of theoretical approaches. Physical Chemistry Chemical Physics, 2015, 17, 13949-13963.	1.3	90
358	Mechanistic Studies of Hydrogen Evolution in Aqueous Solution Catalyzed by a Tertpyridineâ€“Amine Cobalt Complex. Inorganic Chemistry, 2015, 54, 4310-4321.	1.9	64
359	Experimental evidence suggesting that H₂O₂ is produced within the thylakoid membrane in a reaction between plastoquinol and singlet oxygen. FEBS Letters, 2015, 589, 779-786.	1.3	40
360	Ionâ€“dipole interactions and their functions in proteins. Protein Science, 2015, 24, 1040-1046.	3.1	41
361	Examining the selectivity of borohydride for carbon dioxide and bicarbonate reduction in protic conditions. Fuel, 2015, 150, 139-145.	3.4	34
362	Electrocatalytic Water Oxidation by a Water-Soluble Nickel Porphyrin Complex at Neutral pH with Low Overpotential. Inorganic Chemistry, 2015, 54, 5604-5613.	1.9	247
363	Silverâ€“Water Clusters: A Theoretical Description of Ag_n(H₂O)_m for n = 1â€“4; m = 1â€“4. Journal of Physical Chemistry C, 2015, 119, 8299-8309.	1.5	7
364	Predicting accurate absolute binding energies in aqueous solution: thermodynamic considerations for electronic structure methods. Physical Chemistry Chemical Physics, 2015, 17, 12441-12451.	1.3	108
365	Predicting Stability Constants for Uranyl Complexes Using Density Functional Theory. Inorganic Chemistry, 2015, 54, 3995-4001.	1.9	83
366	Using computational chemistry to design Ru photosensitizers with directional charge transfer. Coordination Chemistry Reviews, 2015, 304-305, 146-165.	9.5	55
367	Absolute BrÃ¸nsted Acidities and pH Scales in Ionic Liquids. ChemPhysChem, 2015, 16, 1428-1439.	1.0	23
368	Computational modelling of gold complexes using density functional theory. Computational and Theoretical Chemistry, 2015, 1073, 45-54.	1.1	12
369	Photochemistry of 4-Chlorophenol in Liquid and Frozen Aqueous Media Studied by Chemical, Compound-Specific Isotope, and DFT Analyses. Langmuir, 2015, 31, 10743-10750.	1.6	17

#	Article	IF	Citations
370	The thermodynamics and biodegradability of chelating agents upon metal extraction. Chemical Engineering Science, 2015, 137, 768-785.	1.9	17
371	Spicing up continuum solvation models with SaLSA: The spherically averaged liquid susceptibility ansatz. Journal of Chemical Physics, 2015, 142, 054102.	1.2	48
372	Theoretical Investigation of a Parallel Catalytic Cycle in CO₂ Hydrogenation by (PNP)IrH₃. Organometallics, 2015, 34, 4932-4940.	1.1	38
373	Ab Initio Molecular Dynamics Simulations of Amino Acids in Aqueous Solutions: Estimating pK_a Values from Metadynamics Sampling. Journal of Physical Chemistry B, 2015, 119, 12249-12255.	1.2	27
374	Six-Electron Reduction of Nitrite to Ammonia by Cytochrome c Nitrite Reductase: Insights from Density Functional Theory Studies. Inorganic Chemistry, 2015, 54, 9303-9316.	1.9	63
375	BF₃-promoted electrochemical properties of quinoxaline in propylene carbonate. RSC Advances, 2015, 5, 18822-18831.	1.7	36
376	Cluster-continuum quasichemical theory calculation of the lithium ion solvation in water, acetonitrile and dimethyl sulfoxide: an absolute single-ion solvation free energy scale. Physical Chemistry Chemical Physics, 2015, 17, 26745-26755.	1.3	54
377	Ab Initio MD Simulations of the BrÃ¸nsted Acidity of Glutathione in Aqueous Solutions: Predicting pK_a Shifts of the Cysteine Residue. Journal of Physical Chemistry B, 2015, 119, 15353-15358.	1.2	40
378	Catalytic Reduction of CO₂ by Renewable Organohydrides. Journal of Physical Chemistry Letters, 2015, 6, 5078-5092.	2.1	59
379	Effect of Stacking Interactions on the Thermodynamics and Kinetics of Lumiflavin: A Study with Improved Density Functionals and Density Functional Tight-Binding Protocol. Journal of Physical Chemistry A, 2015, 119, 172-182.	1.1	13
380	Are thermodynamic cycles necessary for continuum solvent calculation of pK_as and reduction potentials?. Physical Chemistry Chemical Physics, 2015, 17, 2859-2868.	1.3	166
381	Rhodium Bis(quinolinyl)benzene Complexes for Methane Activation and Functionalization. Chemistry - A European Journal, 2015, 21, 1286-1293.	1.7	24
382	A Simple Method for Estimating the Absolute Solvation Free Energy of Monovalent Ions in Different Solvents. Journal of Physical Chemistry A, 2015, 119, 160-171.	1.1	5
383	Calculations of pK_aâ€™s and Redox Potentials of Nucleobases with Explicit Waters and Polarizable Continuum Solvation. Journal of Physical Chemistry A, 2015, 119, 5134-5144.	1.1	111
384	Selfâ€Assembly of Uranylâ€“Peroxide Nanocapsules in Basic Peroxidic Environments. Chemistry - A European Journal, 2016, 22, 8571-8578.	1.7	32
386	Reaction Mechanism and Regioselectivity of the Bingelâ€“Hirsch Addition of Dimethyl Bromomalonate to La@C₂v</sub>â€“₈₂. Chemistry - A European Journal, 2016, 22, 5953-5962.	1.7	23
387	Computational S N 2â€Type Mechanism for the Difluoromethylation of Lithium Enolate with Fluoroform through Bimetallic Câ^'F Bond Dual Activation. Chemistry - A European Journal, 2016, 22, 8796-8800.	1.7	18
388	Experimental Insight into the Thermodynamics of the Dissolution of Electrolytes in Room-Temperature Ionic Liquids: From the Mass Action Law to the Absolute Standard Chemical Potential of a Proton. ACS Omega, 2016, 1, 1393-1411.	1.6	16

#	Article	IF	Citations
389	Quantum Mechanics/Molecular Mechanics Method Combined with Hybrid All-Atom and Coarse-Grained Model: Theory and Application on Redox Potential Calculations. Journal of Chemical Theory and Computation, 2016, 12, 2017-2027.	2.3	18
390	Tuning the Stability of Organic Active Materials for Nonaqueous Redox Flow Batteries via Reversible, Electrochemically Mediated Li⁺ Coordination. Chemistry of Materials, 2016, 28, 2529-2539.	3.2	37
391	Reduced State of Iridium PCP Pincer Complexes in Electrochemical CO₂ Hydrogenation. ACS Catalysis, 2016, 6, 3834-3839.	5.5	23
392	Airâ€“water partition coefficients for a suite of polycyclic aromatic and other C₁₀through C₂₀unsaturated hydrocarbons. Journal of Environmental Science and Health - Part A Toxic/Hazardous Substances and Environmental Engineering, 2016, 51, 938-953.	0.9	2
393	Chemical Forms of Mercury in Human Hair Reveal Sources of Exposure. Environmental Science & Technology, 2016, 50, 10721-10729.	4.6	53
394	Computational Study of the Radical Mediated Mechanism of the Formation of C8, C5, and C4 Guanine:Lysine Adducts in the Presence of the Benzophenone Photosensitizer. Chemical Research in Toxicology, 2016, 29, 1396-1409.	1.7	16
395	Acidity Constant (pK_a) Calculation of Large Solvated Dye Molecules: Evaluation of Two Advanced Molecular Dynamics Methods. ChemPhysChem, 2016, 17, 3447-3459.	1.0	20
396	Selectivity for HCO₂^{â€“} over H₂ in the Electrochemical Catalytic Reduction of CO₂ by (POCOP)IrH₂. ACS Catalysis, 2016, 6, 6362-6371.	5.5	33
397	Multiconformation, Density Functional Theory-Based pK_a Prediction in Application to Large, Flexible Organic Molecules with Diverse Functional Groups. Journal of Chemical Theory and Computation, 2016, 12, 6001-6019.	2.3	108
398	Partition coefficients for the SAMPL5 challenge using transfer free energies. Journal of Computer-Aided Molecular Design, 2016, 30, 1129-1138.	1.3	19
399	Electronegativity and redox reactions. Physical Chemistry Chemical Physics, 2016, 18, 22235-22243.	1.3	42
400	Toward Quantitatively Accurate Calculation of the Redox-Associated Acidâ€“Base and Ligand Binding Equilibria of Aquacobalamin. Journal of Physical Chemistry B, 2016, 120, 7307-7318.	1.2	3
401	Enthalpic and Entropic Contributions to Hydrophobicity. Journal of Chemical Theory and Computation, 2016, 12, 4600-4610.	2.3	68
402	Origin of Acidâ€“Base Catalytic Effects on Formaldehyde Hydration. Journal of Physical Chemistry A, 2016, 120, 9598-9606.	1.1	4
403	Stability of organic compounds on the oxygen-evolving center of photosystem II and manganese oxide water oxidation catalysts. Chemical Communications, 2016, 52, 13760-13763.	2.2	18
404	Theoretical Calculation of pK_aâ€™s of Selenols in Aqueous Solution Using an Implicit Solvation Model and Explicit Water Molecules. Journal of Physical Chemistry A, 2016, 120, 8916-8922.	1.1	38
405	Theoretical inclusion of deprotonated 2,4-D and dicamba pesticides in ÃŸ-cyclodextrin. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 86, 343-349.	0.9	9
406	Cationic CHâ‹Ï€ interactions as a function of solvation. Physical Chemistry Chemical Physics, 2016, 18, 30940-30945.	1.3	18

#	Article	IF	Citations
407	O₂ Activation in Salicylate 1,2-Dioxygenase: A QM/MM Study Reveals the Role of His162. Inorganic Chemistry, 2016, 55, 11727-11735.	1.9	14
408	Electrochemical Stability Window of Imidazolium-Based Ionic Liquids as Electrolytes for Lithium Batteries. Journal of Physical Chemistry B, 2016, 120, 5691-5702.	1.2	182
409	Structure and Stability Studies of Pharmacologically Relevant S-Nitrosothiols: A Theoretical Approach. Journal of Physical Chemistry A, 2016, 120, 4191-4200.	1.1	18
410	Computing pK_a Values in Different Solvents by Electrostatic Transformation. Journal of Chemical Theory and Computation, 2016, 12, 3360-3369.	2.3	28
411	Density Functional Theory Calculation of pK_aâ€™s of Thiols in Aqueous Solution Using Explicit Water Molecules and the Polarizable Continuum Model. Journal of Physical Chemistry A, 2016, 120, 5726-5735.	1.1	146
412	Molecular Level Understanding of the Factors Affecting the Stability of Dimethoxy Benzene Catholyte Candidates from First-Principles Investigations. Journal of Physical Chemistry C, 2016, 120, 14531-14538.	1.5	33
413	Entrapment of Cyclic Fluorideâ€“Water and Sulfateâ€“Waterâ€“Sulfate Cluster Within the Self-Assembled Structure of Linear meta-Phenylenediamine Based Bis-Urea Receptors: Positional Isomeric Effect. Crystal Growth and Design, 2016, 16, 2893-2903.	1.4	28
414	Rational Design of Methodology-Independent Metal Parameters Using a Nonbonded Dummy Model. Journal of Chemical Theory and Computation, 2016, 12, 3250-3260.	2.3	40
415	Substituent effect on the proton-related phenomena and chelation behavior of hydroxypicolinic compounds: a DFT investigation. Structural Chemistry, 2016, 27, 505-524.	1.0	4
416	Theoretical study on Pd-catalyzed reaction of aryl iodide with unsymmetrical alkyne. Journal of Organometallic Chemistry, 2016, 803, 134-141.	0.8	4
417	Hydration Free Energies of Molecular Ions from Theory and Simulation. Journal of Physical Chemistry B, 2016, 120, 975-983.	1.2	63
418	Multigrid-Based Methodology for Implicit Solvation Models in Periodic DFT. Journal of Chemical Theory and Computation, 2016, 12, 1331-1341.	2.3	61
419	LiCl solvation in N-methyl-acetamide (NMA) as a model for understanding Li⁺binding to an amide plane. Physical Chemistry Chemical Physics, 2016, 18, 4191-4200.	1.3	23
420	In Vivo Detection of Mitochondrial Dysfunction Induced by Clinical Drugs and Disease-Associated Genes Using a Novel Dye ZMJ214 in Zebrafish. ACS Chemical Biology, 2016, 11, 381-388.	1.6	16
421	Isodesmic reaction for accurate theoretical pK_a calculations of amino acids and peptides. Physical Chemistry Chemical Physics, 2016, 18, 11202-11212.	1.3	35
422	Quantum chemical approach for condensed-phase thermochemistry (III): Accurate evaluation of proton hydration energy and standard hydrogen electrode potential. Chemical Physics Letters, 2016, 650, 159-164.	1.2	24
423	Exploration of the Detailed Conditions for Reductive Stability of Mg(TFSI)₂ in Diglyme: Implications for Multivalent Electrolytes. Journal of Physical Chemistry C, 2016, 120, 3583-3594.	1.5	81
424	A density functional theory protocol for the calculation of redox potentials of copper complexes. Physical Chemistry Chemical Physics, 2016, 18, 5529-5536.	1.3	42

#	Article	IF	Citations
425	Azide Binding Controlled by Steric Interactions in Second Sphere. Synthesis, Crystal Structure, and Magnetic Properties of [Ni^{II}₂(L)(Î¼_{1,1}-N₃)][ClO₄] (L = Macrocyclic) Tj ETQq0 0 0 rgBT /Overl	1.9	15
426	Theoretical study on Au(<scp>i</scp>)-catalyzed [2 + 2 + 2] cycloadditions of ynamides with two discrete nitriles. Organic and Biomolecular Chemistry, 2016, 14, 2637-2644.	1.5	16
427	Pair correlations that link the hydrophobic and Hofmeister effects. Physical Chemistry Chemical Physics, 2016, 18, 14949-14959.	1.3	5
428	Water oxidation catalysis with ligand substituted Ruâ€“bpp type complexes. Catalysis Science and Technology, 2016, 6, 5088-5101.	2.1	23
429	Interconversion of Formic Acid and Carbon Dioxide by Proton-Responsive, Half-Sandwich Cp*Ir^{III} Complexes: A Computational Mechanistic Investigation. ACS Catalysis, 2016, 6, 600-609.	5.5	68
430	Mechanism of Ni-NHC Catalyzed Hydrogenolysis of Aryl Ethers: Roles of the Excess Base. ACS Catalysis, 2016, 6, 483-493.	5.5	76
431	Thermodynamic Parameters Including Acid Dissociation Constants for Bromochlorophenols (BCPs). Journal of Chemical & Engineering Data, 2016, 61, 160-172.	1.0	2
432	Reaction Mechanisms in Carbon Dioxide Conversion. , 2016, , .		70
433	One- and Multi-electron Pathways for the Reduction of CO2 into C1 and C1+ Energy-Richer Molecules: Some Thermodynamic and Kinetic Facts. , 2016, , 311-345.		4
434	Revisiting the solvation enthalpies and free energies of the proton and electron in various solvents. Computational and Theoretical Chemistry, 2016, 1077, 11-17.	1.1	148
435	Single-ion hydration thermodynamics from clusters to bulk solutions: Recent insights from molecular modeling. Fluid Phase Equilibria, 2016, 407, 58-75.	1.4	32
436	Mechanistic Study of the Validity of Using Hydroxyl Radical Probes To Characterize Electrochemical Advanced Oxidation Processes. Environmental Science & Technology, 2017, 51, 2355-2365.	4.6	168
437	Quantum chemical study and isothermal titration calorimetry of Î²-cyclodextrin complexes with mianserin in aqueous solution. Organic and Biomolecular Chemistry, 2017, 15, 1209-1216.	1.5	14
438	Protonation equilibria of transition metal complexes: From model systems toward the Mn-complex in photosystem II. Coordination Chemistry Reviews, 2017, 345, 16-30.	9.5	15
439	Substrate Specificity and Leaving Group Effect in Ester Cleavage by Metal Complexes of an Oximate Nucleophile. Inorganic Chemistry, 2017, 56, 2060-2069.	1.9	5
440	Iridium and Ruthenium Complexes of N-Heterocyclic Carbene- and Pyridinol-Derived Chelates as Catalysts for Aqueous Carbon Dioxide Hydrogenation and Formic Acid Dehydrogenation: The Role of the Alkali Metal. Organometallics, 2017, 36, 1091-1106.	1.1	94
441	Effect of the protein ligand in DMSO reductase studied by computational methods. Journal of Inorganic Biochemistry, 2017, 171, 45-51.	1.5	7
442	Deactivation of a Cobalt Catalyst for Water Reduction through Valence Tautomerism. Chemistry - A European Journal, 2017, 23, 9266-9271.	1.7	14

#	Article	IF	Citations
443	Determination of the real potential of chloride ion in water by using a voltaic cell with a dropping carbon fluid electrode. Journal of Electroanalytical Chemistry, 2017, 797, 42-46.	1.9	1
444	Bimetallic Cooperativity in Proton Reduction with an Amidoâ€Bridged Cobalt Catalyst. Chemistry - A European Journal, 2017, 23, 9272-9279.	1.7	21
445	A theoretical study of ascorbic acid oxidation andHOOË™/O₂Ë™^{â^'}radical scavenging. Organic and Biomolecular Chemistry, 2017, 15, 4417-4431.	1.5	108
446	Silverâ€“Water Clusters: A Computation of Ag_n(H₂O)_m for n = 1â€“6; m = 1â€“8. Journal of Physical Chemistry C, 2017, 121, 11811-11823.	1.5	7
447	Phenol-Induced Oâ€“O Bond Cleavage in a Low-Spin Hemeâ€“Peroxoâ€“Copper Complex: Implications for O₂ Reduction in Hemeâ€“Copper Oxidases. Journal of the American Chemical Society, 2017, 139, 7958-7973.	6.6	43
448	Computational study of Th4+ and Np4+ hydration and hydrolysis of Th4+ from first principles. Journal of Molecular Modeling, 2017, 23, 69.	0.8	5
449	DFT study of structural and electronic properties of gallic acid and its anions in gas phase and in aqueous solution. Structural Chemistry, 2017, 28, 1789-1802.	1.0	31
450	DFT Studies of Ru-Catalyzed Câ€“O versus Câ€“H Bond Functionalization of Aryl Ethers with Organoboronates. Organometallics, 2017, 36, 2354-2363.	1.1	20
451	A computational study of the main degradation product of antitumor drug imexon. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750037.	1.8	0
452	Electrocatalytic Water Oxidation by a Homogeneous Copper Catalyst Disfavors Single-Site Mechanisms. Journal of the American Chemical Society, 2017, 139, 8586-8600.	6.6	107
453	Improved pK_a Prediction of Substituted Alcohols, Phenols, and Hydroperoxides in Aqueous Medium Using Density Functional Theory and a Cluster-Continuum Solvation Model. Journal of Physical Chemistry A, 2017, 121, 4698-4706.	1.1	77
454	Free-Energy Calculations of Ionic Hydration Consistent with the Experimental Hydration Free Energy of the Proton. Journal of Physical Chemistry Letters, 2017, 8, 2705-2712.	2.1	40
455	Intramolecular Oxyl Radical Coupling Promotes Oâ€“O Bond Formation in a Homogeneous Mononuclear Mn-based Water Oxidation Catalyst: A Computational Mechanistic Investigation. Inorganic Chemistry, 2017, 56, 4435-4445.	1.9	35
456	Dihydropteridine/Pteridine as a 2H⁺/2e^{â€“} Redox Mediator for the Reduction of CO₂ to Methanol: A Computational Study. Journal of Physical Chemistry B, 2017, 121, 4158-4167.	1.2	13
457	Solvation energies of the proton in ammonia explicitly versus temperature. Journal of Chemical Physics, 2017, 146, 134308.	1.2	36
458	Extraction Behaviors of Heavy Rare Earths with Organophosphoric Extractants: The Contribution of Extractant Dimer Dissociation, Acid Ionization, and Complexation. A Quantum Chemistry Study. Journal of Physical Chemistry A, 2017, 121, 2531-2543.	1.1	35
459	Theoretical pK prediction of the Î±-phosphate moiety of uridine 5â€²-diphosphate-GlcNAc. Chemical Physics Letters, 2017, 667, 220-225.	1.2	7
460	QSARs for phenols and phenolates: oxidation potential as a predictor of reaction rate constants with photochemically produced oxidants. Environmental Sciences: Processes and Impacts, 2017, 19, 324-338.	1.7	44

#	Article	IF	Citations
461	Mechanism of the OH Radical Addition to Adenine from Quantum-Chemistry Determinations of Reaction Paths and Spectroscopic Tracking of the Intermediates. Journal of Organic Chemistry, 2017, 82, 276-288.	1.7	20
462	Level Alignment as Descriptor for Semiconductor/Catalyst Systems in Water Splitting: The Case of Hematite/Cobalt Hexacyanoferrate Photoanodes. ChemSusChem, 2017, 10, 4552-4560.	3.6	33
463	Comparative Assessment of Computational Methods for Free Energy Calculations of Ionic Hydration. Journal of Chemical Information and Modeling, 2017, 57, 2763-2775.	2.5	20
464	Electrocatalytic Water Oxidation by a Water-Soluble Copper(II) Complex with a Copper-Bound Carbonate Group Acting as a Potential Proton Shuttle. Inorganic Chemistry, 2017, 56, 13368-13375.	1.9	81
465	Electrostatic solvation free energies of charged hard spheres using molecular dynamics with density functional theory interactions. Journal of Chemical Physics, 2017, 147, 161716.	1.2	42
466	Study of interactions between metal ions and protein model compounds by energy decomposition analyses and the AMOEBA force field. Journal of Chemical Physics, 2017, 147, 161733.	1.2	48
467	Why can a gold salt react as a base?. Organic and Biomolecular Chemistry, 2017, 15, 7841-7852.	1.5	6
468	Increase in Solubility of Poorly-Ionizable Pharmaceuticals by Salt Formation: A Case of Agomelatine Sulfonates. Crystal Growth and Design, 2017, 17, 5283-5294.	1.4	13
469	Crystal nucleation initiated by transient ion-surface interactions at aerosol interfaces. Science Advances, 2017, 3, e1700425.	4.7	16
470	Intramolecular S_EAr Reactions of Phosphorus Compounds: Computational Approach to the Synthesis of Ï€â€Extended Heterocycles. Chemistry - A European Journal, 2017, 23, 17487-17496.	1.7	14
471	Organic ion association in aqueous phase and ab initio-based force fields: The case of carboxylate/ammonium salts. Journal of Chemical Physics, 2017, 147, 161720.	1.2	9
472	First-Principles Molecular Dynamics Analysis of Ligand-Free Suzukiâ€“Miyaura Cross-Coupling in Water: Transmetalation and Reductive Elimination. Journal of Physical Chemistry C, 2017, 121, 19904-19914.	1.5	9
473	Assessment of Methodology and Chemical Group Dependences in the Calculation of the pK_a for Several Chemical Groups. Journal of Chemical Theory and Computation, 2017, 13, 4791-4803.	2.3	25
474	Substituent, Charge, and Size Effects on the Fluorogenic Performance of Amyloid Ligands: A Small-Library Screening Study. ACS Omega, 2017, 2, 3192-3200.	1.6	19
475	Real single ion solvation free energies with quantum mechanical simulation. Chemical Science, 2017, 8, 6131-6140.	3.7	63
476	Targeting the reactive intermediate in polysaccharide monooxygenases. Journal of Biological Inorganic Chemistry, 2017, 22, 1029-1037.	1.1	52
477	Absolute ion hydration enthalpies and the role of volume within hydration thermodynamics. RSC Advances, 2017, 7, 27881-27894.	1.7	26
478	Protonation States of Homocitrate and Nearby Residues in Nitrogenase Studied by Computational Methods and Quantum Refinement. Journal of Physical Chemistry B, 2017, 121, 8242-8262.	1.2	62

#	Article	IF	Citations
479	A unified view to BrÃ¸nsted acidity scales: do we need solvated protons?. Chemical Science, 2017, 8, 6964-6973.	3.7	59
480	Complexation of Al³⁺ and Ni²⁺ by <scp>l</scp>-Ascorbic Acid: An Experimental and Theoretical Investigation. Journal of Physical Chemistry A, 2017, 121, 9773-9781.	1.1	21
481	Structure and Bonding in Uranyl(VI) Peroxide and Crown Ether Complexes; Comparison of Quantum Chemical and Experimental Data. Inorganic Chemistry, 2017, 56, 15231-15240.	1.9	5
482	Variational transition state theory: theoretical framework and recent developments. Chemical Society Reviews, 2017, 46, 7548-7596.	18.7	281
483	Design, synthesis and multitarget biological profiling of second-generation anti-Alzheimer rheinâ€“huprine hybrids. Future Medicinal Chemistry, 2017, 9, 965-981.	1.1	40
484	Prediction of Mass Spectral Response Factors from Predicted Chemometric Data for Druglike Molecules. Journal of the American Society for Mass Spectrometry, 2017, 28, 278-285.	1.2	12
485	Determination of acidic constants of tetrafluoro-p-hydroquinone. Journal of Fluorine Chemistry, 2017, 193, 33-37.	0.9	1
486	Developing multisite empirical force field models for Pt(II) and cisplatin. Journal of Computational Chemistry, 2017, 38, 161-168.	1.5	5
487	The Determination of Absolute Values of Entropies of Hydration [Î”Sabs0(H+)h]$[Delta S_{abs}^0{({H^) Tj ETQq0 0 0 rgBT /Overlock 1 Proton in Solutions. Zeitschrift Fur Physikalische Chemie, 2017, 231, 983-1015.	1.4	5
488	Twoâ€State Reactivity of Histone Demethylases Containing Jumonjiâ€C Active Sites: Different Mechanisms for Different Methylation Degrees. Chemistry - A European Journal, 2017, 23, 137-148.	1.7	13
489	Determination of the Bridging Ligand in the Active Site of Tyrosinase. Molecules, 2017, 22, 1836.	1.7	14
490	Carbonate and carbonate anion radicals in aqueous solutions exist as CO₃(H₂O)₆^{2â^’} and CO₃(H₂O)₆Ë™^{â^’} respectively: the crucial role of the inner hydration sphere of anions in explaining their properties. Physical Chemistry Chemical Physics, 2018, 20, 9429-9435.	1.3	26
491	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. Journal of Chemical Information and Modeling, 2018, 58, 993-1004.	2.5	45
492	Resolving Confined ⁷Li Dynamics of Uranyl Peroxide Capsule U₂₄. Inorganic Chemistry, 2018, 57, 5514-5525.	1.9	10
493	Flexible proton-responsive ligand-based Mn(<scp>i</scp>) complexes for CO₂ hydrogenation: a DFT study. Physical Chemistry Chemical Physics, 2018, 20, 12535-12542.	1.3	11
494	Quantum Chemical Calculation of pK_as of Environmentally Relevant Functional Groups: Carboxylic Acids, Amines, and Thiols in Aqueous Solution. Journal of Physical Chemistry A, 2018, 122, 4366-4374.	1.1	62
495	Quantum Chemistry Study on the Extraction of Trivalent Lanthanide Series by Cyanex301: Insights from Formation of Inner- and Outer-Sphere Complexes. ACS Omega, 2018, 3, 4070-4080.	1.6	17
496	Comparative CHARMM and AMOEBA Simulations of Lanthanide Hydration Energetics and Experimental Aqueous-Solution Structures. Journal of Chemical Theory and Computation, 2018, 14, 1781-1790.	2.3	28

#	Article	IF	Citations
497	Empirical Conversion of pK_a Values between Different Solvents and Interpretation of the Parameters: Application to Water, Acetonitrile, Dimethyl Sulfoxide, and Methanol. ACS Omega, 2018, 3, 1653-1662.	1.6	92
498	Quest for Organic Active Materials for Redox Flow Batteries: 2,3-Diaza-anthraquinones and Their Electrochemical Properties. Chemistry of Materials, 2018, 30, 762-774.	3.2	44
499	Theoretical study on the reaction mechanism of Pd(OAc)2-catalyzed trifluoroethylation: Role of additive CF3COOH. Tetrahedron Letters, 2018, 59, 462-468.	0.7	6
500	Quantum Chemical Prediction of pK_a Values of Cationic Ion-Exchange Groups in Polymer Electrolyte Membranes. Journal of Physical Chemistry C, 2018, 122, 2490-2501.	1.5	14
501	Calculation of Reaction Free Energies in Solution: A Comparison of Current Approaches. Journal of Physical Chemistry A, 2018, 122, 1392-1399.	1.1	101
502	pK_a Prediction. , 2018, , 503-518.		0
503	Computational Electrochemistry as a Reliable Probe of Experimentally Elusive Mononuclear Nonheme Iron Species. Journal of Physical Chemistry C, 2018, 122, 10773-10782.	1.5	12
504	Structural characterization of the P1+ intermediate state of the P-cluster of nitrogenase. Journal of Biological Chemistry, 2018, 293, 9629-9635.	1.6	44
505	Theoretical Studies of the Formation Mechanisms, Thermodynamic Stabilities, and Water-Exchange Reactivities of Aluminum-Salicylate Complexes in Aqueous Solution. ACS Earth and Space Chemistry, 2018, 2, 422-431.	1.2	5
506	Absolute proton hydration free energy, surface potential of water, and redox potential of the hydrogen electrode from first principles: QM/MM MD free-energy simulations of sodium and potassium hydration. Journal of Chemical Physics, 2018, 148, 222814.	1.2	71
507	Basic Remarks on Acidity. Angewandte Chemie - International Edition, 2018, 57, 4386-4411.	7.2	48
508	Axial baseâ€controlled catalytic activity, oxidative stability and product selectivity of waterâ€insoluble manganese and iron porphyrins for oxidation of styrenes in water under green conditions. Applied Organometallic Chemistry, 2018, 32, e4117.	1.7	8
509	Thermodynamics of aqueous perfluorooctanoic acid (PFOA) and 4,8-dioxa-3H-perfluorononanoic acid (DONA) from DFT calculations: Insights into degradation initiation. Chemosphere, 2018, 193, 1063-1070.	4.2	20
510	Grundlegende Bemerkungen zur AziditÃt. Angewandte Chemie, 2018, 130, 4471-4498.	1.6	13
511	Solvation energies of the proton in methanol revisited and temperature effects. Physical Chemistry Chemical Physics, 2018, 20, 29184-29206.	1.3	54
512	Precise estimation of transfer free energies for ionic species between similar media. Physical Chemistry Chemical Physics, 2018, 20, 27003-27010.	1.3	1
513	Combining Experiment and Theory To Unravel the Mechanism of Two-Electron Oxygen Reduction at a Selective and Active Co-catalyst. ACS Catalysis, 2018, 8, 11940-11951.	5.5	45
514	Thermochemical parameters of chlorinated compounds of pyridine. Computational and Theoretical Chemistry, 2018, 1146, 21-26.	1.1	1

#	Article	IF	Citations
515	Cyclic Changes in Active Site Polarization and Dynamics Drive the â€œPing-pongâ€•Kinetics in NRH:Quinone Oxidoreductase 2: An Insight from QM/MM Simulations. ACS Catalysis, 2018, 8, 12015-12029.	5.5	7
516	Dopamine Autoxidation Is Controlled by Acidic pH. Frontiers in Molecular Neuroscience, 2018, 11, 467.	1.4	81
517	Renewable Hydride Donors for the Catalytic Reduction of CO₂: A Thermodynamic and Kinetic Study. Journal of Physical Chemistry B, 2018, 122, 10179-10189.	1.2	13
518	Electrochemical Oxidation of Atrazine and Clothianidin on Bi-doped SnO₂â€“Ti_nO_{2nâ€“1} Electrocatalytic Reactive Electrochemical Membranes. Environmental Science & Technology, 2018, 52, 12675-12684.	4.6	127
519	A Theoretical Study on Redox Potential and pKa of [2Fe-2S] Cluster Model from Iron-Sulfur Proteins. Bulletin of the Chemical Society of Japan, 2018, 91, 1451-1456.	2.0	4
520	Single-Ion Thermodynamics from First Principles: Calculation of the Absolute Hydration Free Energy and Single-Electrode Potential of Aqueous Li⁺ Using ab Initio Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 6443-6459.	2.3	18
521	Superhalogen-based composite with strong acidity-a crossing point between two topics. Inorganic Chemistry Frontiers, 2018, 5, 2934-2947.	3.0	17
522	Stereoselectivity, Different Oxidation States, and Multiple Spin States in the Cyclopropanation of Olefins Catalyzed by Feâ€“Porphyrin Complexes. ACS Catalysis, 2018, 8, 11140-11153.	5.5	27
523	Quantum Chemical Approach for Calculating Stability Constants of Mercury Complexes. ACS Earth and Space Chemistry, 2018, 2, 1168-1178.	1.2	14
524	Thermochemically Consistent Free Energies of Hydration for Di- and Trivalent Metal Ions. Journal of Physical Chemistry A, 2018, 122, 7464-7471.	1.1	14
525	Mechanisms and stereoselectivities of phosphineâ€catalyzed (3+3) cycloaddition reaction between azomethine imine and ynone: A computational study. International Journal of Quantum Chemistry, 2018, 118, e25729.	1.0	1
526	Improving solvation energy predictions using the SMD solvation method and semiempirical electronic structure methods. Journal of Chemical Physics, 2018, 149, 104102.	1.2	39
527	A Reaction Mechanism for Gold-Catalyzed Hydroamination/Cyclization of o-Phenylendiamine and Propargylic Alcohols. A DFT Study. Organometallics, 2018, 37, 3035-3044.	1.1	8
528	Stability constants of Cu(II)/indomethacin mononuclear complexes in solution. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	5
529	Refined SMD Parameters for Bromine and Iodine Accurately Model Halogenâ€Bonding Interactions in Solution. Chemistry - A European Journal, 2018, 24, 15983-15987.	1.7	52
530	Cerium Metalâ€“Organic Framework for Photocatalysis. Journal of the American Chemical Society, 2018, 140, 7904-7912.	6.6	313
531	Absolute Energy Levels of Liquid Water. Journal of Physical Chemistry Letters, 2018, 9, 3212-3216.	2.1	51
532	Microkinetic modeling in homogeneous catalysis. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1372.	6.2	85

#	Article	IF	Citations
533	Immobilization of an Amphiphilic Molecular Cobalt Catalyst on Carbon Black for Ligand-Assisted Water Oxidation. Inorganic Chemistry, 2018, 57, 9748-9756.	1.9	18
534	Theoretical study on the acidities of pyrrole, indole, carbazole and their hydrocarbon analogues in DMSO. Canadian Journal of Chemistry, 2018, 96, 1001-1009.	0.6	4
535	Quantum-chemical simulations of the hydration of Pb(II) ion: structure, hydration energies, and pKa1 value. Journal of Molecular Modeling, 2018, 24, 193.	0.8	12
536	Catalytic effects of p-phenylene-bridged methylated binuclear ferrocenes on thermal decomposition of the main component of composite solid propellants. Thermochimica Acta, 2018, 666, 181-189.	1.2	32
537	Hybrid DFT study on non-covalent interactions and their influence on pKa's of magnesium-carboxylate complexes. Journal of Molecular Graphics and Modelling, 2018, 85, 13-24.	1.3	5
538	Quantum Chemical Study of the Redox Potential of the Co(OH2)62+/3+ Couple and the Singletâ€“Quintet Gibbs Energy Difference of the Co(OH2)63+ Ion. Inorganic Chemistry, 2018, 57, 10122-10127.	1.9	1
539	Water-Nucleophilic Attack Mechanism for the Cu^{II}(pyalk)₂ Water-Oxidation Catalyst. ACS Catalysis, 2018, 8, 7952-7960.	5.5	37
540	Re-examining the tetraphenyl-arsonium/tetraphenyl-borate (TATB) hypothesis for single-ion solvation free energies. Journal of Chemical Physics, 2018, 148, 222830.	1.2	22
541	Mechanistic Role of Two-State Reactivity in a Molecular MoS₂ Edge-Site Analogue for Hydrogen Evolution Electrocatalysis. Inorganic Chemistry, 2018, 57, 9167-9174.	1.9	4
542	Understanding the scale of the single ion free energy: A critical test of the tetra-phenyl arsonium and tetra-phenyl borate assumption. Journal of Chemical Physics, 2018, 148, 222819.	1.2	18
543	Influence of intrinsic and extrinsic factors on the antiradical activity of Gallic acid: a theoretical study. Structural Chemistry, 2018, 29, 359-373.	1.0	12
544	One-Electron Reduction Potentials: Calibration of Theoretical Protocols for Moritaâ€“Baylisâ€“Hillman Nitroaromatic Compounds in Aprotic Media. Molecules, 2018, 23, 2129.	1.7	3
545	Square planar or octahedral after all? The indistinct solvation of platinum(ii). Dalton Transactions, 2018, 47, 13032-13045.	1.6	3
546	Tuning the Redox Potentials and Ligand Field Strength of Fe(II) Polypyridines: The Dual Ï€-Donor and Ï€-Acceptor Character of Bipyridine. Inorganic Chemistry, 2018, 57, 9907-9917.	1.9	44
547	Novel 8-nitroquinolin-2(1H)-ones as NTR-bioactivated antikinetoplastid molecules: Synthesis, electrochemical and SAR study. European Journal of Medicinal Chemistry, 2018, 155, 135-152.	2.6	19
548	New hybrid cluster-continuum model for pKa values calculations: Case study of neurotransmittersâ€™ amino group acidity. Chemical Physics, 2019, 516, 55-62.	0.9	7
549	Theoretical Study of the Mechanisms of Two Copper Water Oxidation Electrocatalysts with Bipyridine Ligands. ACS Catalysis, 2019, 9, 8798-8809.	5.5	9
550	Crown Ethers as Electrolyte Additives To Modulate the Electrochemical Potential of Lithium Organic Batteries. Journal of Physical Chemistry C, 2019, 123, 21950-21958.	1.5	6

#	Article	IF	Citations
551	Mechanisms of phosphine-catalyzed [3+3] cycloaddition of ynones and azomethine imines: a DFT study. New Journal of Chemistry, 2019, 43, 13600-13607.	1.4	10
552	Acidâ€“Base Equilibria. , 2019, , 17-91.		2
553	Improving Performance of the SMD Solvation Model: Bondi Radii Improve Predicted Aqueous Solvation Free Energies of Ions and pK_a Values of Thiols. Journal of Physical Chemistry A, 2019, 123, 9498-9504.	1.1	37
554	A multicomponent synthesis of stereodefined olefins via nickel catalysis and single electron/triplet energy transfer. Nature Catalysis, 2019, 2, 678-687.	16.1	123
555	Examining the Factors That Govern the Regioselectivity in Rhodium-Catalyzed Alkyne Cyclotrimerization. Organometallics, 2019, 38, 2853-2862.	1.1	34
556	â€œIon Solvation Spectraâ€: Free Energy Analysis of Solvation Structures of Multivalent Cations in Aprotic Solvents. Journal of Physical Chemistry Letters, 2019, 10, 4920-4928.	2.1	25
557	A Modified Cationic Mechanism for PdCl2-Catalyzed Transformation of a Homoallylic Alcohol to an Allyl Ether. Organometallics, 2019, 38, 2953-2962.	1.1	10
558	Free Energies of Hydration for Metal Ions from Heats of Vaporization. Journal of Physical Chemistry A, 2019, 123, 6536-6546.	1.1	12
559	Accurate pK_a Evaluations for Complex Bio-Organic Molecules in Aqueous Media. Journal of Chemical Theory and Computation, 2019, 15, 6025-6035.	2.3	31
560	Computational Ag/AgCl Reference Electrode from Density Functional Theory-Based Molecular Dynamics. Journal of Physical Chemistry B, 2019, 123, 10224-10232.	1.2	15
561	Ion hydration free energies and water surface potential in water nano drops: The cluster pair approximation and the proton hydration Gibbs free energy in solution. Journal of Chemical Physics, 2019, 151, 174504.	1.2	9
562	Predicting Potential Inversion Behavior of Ruâ€“aqua Complexes via Using Cost Effective DFT Calculations. Bulletin of the Korean Chemical Society, 2019, 40, 1098-1111.	1.0	1
563	Using N-Terminal Coordination of Cu(II) and Ni(II) to Isolate the Coordination Environment of Cu(I) and Cu(II) Bound to His13 and His14 in Amyloid-Î²(4â€“16). Inorganic Chemistry, 2019, 58, 15138-15154.	1.9	16
564	Improving the Accuracy of PCM-UAHF and PCM-UAKS Calculations Using Optimized Electrostatic Scaling Factors. Journal of Chemical Theory and Computation, 2019, 15, 6958-6967.	2.3	11
565	Computational Study of the Oxidation of Guanine To Form 5-Carboxyamido-5-formamido-2-iminohydantoin (2Ih). Chemical Research in Toxicology, 2019, 32, 2295-2304.	1.7	6
566	QresFEP: An Automated Protocol for Free Energy Calculations of Protein Mutations in Q. Journal of Chemical Theory and Computation, 2019, 15, 5461-5473.	2.3	33
567	Ultrafast Proton Transport between a Hydroxy Acid and a Nitrogen Base along Solvent Bridges Governed by the Hydroxide/Methoxide Transfer Mechanism. Journal of the American Chemical Society, 2019, 141, 14581-14592.	6.6	26
568	Density Functional Calculations for Aqueous Silver Clusters Containing Water and Nitrate Ligands. Journal of Physical Chemistry B, 2019, 123, 8300-8312.	1.2	0

#	Article	IF	Citations
569	Radical-Stimulated Nucleophile Release. Journal of Organic Chemistry, 2019, 84, 12606-12616.	1.7	2
570	Understanding Carbamate Formation Reaction Thermochemistry of Amino Acids as Solvents for Postcombustion CO₂ Capture. Journal of Physical Chemistry B, 2019, 123, 8433-8447.	1.2	13
571	An Investigation of Electrocatalytic CO2 Reduction Using a Manganese Tricarbonyl Biquinoline Complex. Frontiers in Chemistry, 2019, 7, 628.	1.8	26
572	Unravelling the Reaction Mechanism of Formic Acid Dehydrogenation by Cp*Rh(III) and Cp*Co(III) Catalysts with Proton-Responsive 4,4â€²- and 6,6â€²-Dihydroxy-2,2â€²-Bipyridine Ligands: A DFT Study. Journal of Physical Chemistry C, 2019, 123, 25061-25073.	1.5	12
573	Designing air-stable cyclometalated Fe(<scp>ii</scp>) complexes: stabilization via electrostatic effects. Dalton Transactions, 2019, 48, 374-378.	1.6	12
574	Constructing organic superacids from superhalogens is a rational route as verified by DFT calculations. Physical Chemistry Chemical Physics, 2019, 21, 2804-2815.	1.3	15
575	The chemical reactions in electrosprays of water do not always correspond to those at the pristine airâ€“water interface. Chemical Science, 2019, 10, 2566-2577.	3.7	43
576	Exploring chemical speciation at electrified interfaces using detailed continuum models. Journal of Chemical Physics, 2019, 150, 041725.	1.2	13
577	Solvent effect on Al(III) hydrolysis constants from density functional theory. Molecular Physics, 2019, 117, 1507-1518.	0.8	0
578	Proton transfer from pinene stabilizes water clusters. Physical Chemistry Chemical Physics, 2019, 21, 13925-13933.	1.3	5
579	On the â€œBornâ€•term used in thermodynamic models for electrolytes. Journal of Chemical Physics, 2019, 150, 244503.	1.2	22
580	On the Miscibility and Immiscibility of Ionic Liquids and Water. Journal of Physical Chemistry B, 2019, 123, 5343-5356.	1.2	29
581	Computational Study of the Formation of C8, C5, and C4 Guanine:Lysine Adducts via Oxidation of Guanine by Sulfate Radical Anion. Journal of Physical Chemistry A, 2019, 123, 5150-5163.	1.1	7
582	Palladium(II) Ion Mediated Disulfide/Thiolate Interconversion: Predicting the Disulfide Group State from First Principles. Journal of Physical Chemistry A, 2019, 123, 4873-4882.	1.1	7
583	DFT Study on the Mechanism of Palladium(0)-Catalyzed Reaction of Aryl Iodides, Norbornene, and Di-tert-butyldiaziridinone. Organometallics, 2019, 38, 2189-2198.	1.1	14
584	Unravelling the reaction mechanism for the Claisenâ€“Tishchenko condensation catalysed by Mn(I)-PNN complexes: a DFT study. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	5
585	QligFEP: an automated workflow for small molecule free energy calculations in Q. Journal of Cheminformatics, 2019, 11, 26.	2.8	51
586	Fate of cisplatin and its main hydrolysed forms in the presence of thiolates: a comprehensive computational and experimental study. Metallomics, 2019, 11, 833-844.	1.0	8

#	Article	IF	Citations
587	Oxidative decomposition mechanisms of lithium peroxide clusters: an Ab Initio study. Molecular Physics, 2019, 117, 1459-1468.	0.8	1
588	Theoretical modeling of pKa's of thiol compounds in aqueous solution. New Journal of Chemistry, 2019, 43, 5239-5254.	1.4	15
589	Water Facilitated Electrochemical Reduction of CO₂ on Cobalt-Porphyrin Catalysts. Journal of Physical Chemistry C, 2019, 123, 9944-9948.	1.5	16
590	Câ€“F activation of perfluorophenazine at nickel: selectivity and mechanistic investigations. Dalton Transactions, 2019, 48, 6153-6161.	1.6	4
591	Nanohybrid sensor for simple, cheap, and sensitive electrochemical recognition and detection of methylglyoxal as chemical markers. Journal of Electroanalytical Chemistry, 2019, 839, 177-186.	1.9	11
592	The multiple dissociation constants of glutathione disulfide: interpreting experimental pH-titration curves with ab initio MD simulations. Physical Chemistry Chemical Physics, 2019, 21, 9212-9217.	1.3	6
593	On the mechanism of protein supercharging in electrospray ionisation mass spectrometry: Effects on charging of additives with short- and long-chain alkyl constituents with carbonate and sulphite terminal groups. Analytica Chimica Acta: X, 2019, 1, 100004.	2.8	8
594	A computational study on the electrified Pt(111) surface by the cluster model. Physical Chemistry Chemical Physics, 2019, 21, 6112-6125.	1.3	9
595	A simple, parameter-free method for computing solvation free energies of ions. Journal of Chemical Physics, 2019, 150, 065101.	1.2	1
596	Catalytic H₂ Evolution by a Mononuclear Cobalt Complex with a Macrocyclic Pentadentate Ligand. European Journal of Inorganic Chemistry, 2019, 2019, 2134-2139.	1.0	14
597	Combining proton and silaborane-based superhalogen anions â€“ an effective route to new superacids as verified via systematic DFT calculations. Dalton Transactions, 2019, 48, 16184-16198.	1.6	9
598	5-Fluorouracilâ€”Complete Insight into Its Neutral and Ionised Forms. Molecules, 2019, 24, 3683.	1.7	41
599	Thiols in Natural Organic Matter: Molecular Forms, Acidity, and Reactivity with Mercury(II) from First-Principles Calculations and High Energy-Resolution X-ray Absorption Near-Edge Structure Spectroscopy. ACS Earth and Space Chemistry, 2019, 3, 2795-2807.	1.2	9
600	Computational Study of the pH-Dependent Competition between Carbonate and Thymine Addition to the Guanine Radical. Chemical Research in Toxicology, 2019, 32, 195-210.	1.7	9
601	On the Use of Thermodynamic Cycles for the Calculation of Standard Potentials for the Oxidation of Solid Metals in Solution. ChemPhysChem, 2019, 20, 159-162.	1.0	0
602	Insight into the structures and reactivities of aqueous Al(III)-carboxylate complexes from cluster-based ab initio computational studies â€“ Implications for the ligand-promoted mineral dissolution mechanism. Geochimica Et Cosmochimica Acta, 2019, 244, 451-466.	1.6	2
603	New Hybrid Method for the Calculation of the Solvation Free Energy of Small Molecules in Aqueous Solutions. Journal of Chemical Theory and Computation, 2019, 15, 371-381.	2.3	14
604	Drug-like properties and complete physicochemical profile of pyrazineâ€2â€amidoxime: A combined multi-experimental and computational studies. Journal of Molecular Liquids, 2019, 276, 453-470.	2.3	13

#	Article	IF	Citations
605	Synergistic Metalâ€“Ligand Redox Cooperativity for Electrocatalytic CO₂ Reduction Promoted by a Ligand-Based Redox Couple in Mn and Re Tricarbonyl Complexes. Organometallics, 2019, 38, 1317-1329.	1.1	37
606	Impact of the redox state of flavin chromophores on the UVâ€“vis spectra, redox and acidity constants and electron affinities. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 387, 112164.	2.0	21
607	Hybrid discreteâ€“continuum solvation methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1440.	6.2	65
608	Persulfate activation induced by ascorbic acid for efficient organic pollutants oxidation. Chemical Engineering Journal, 2020, 382, 122355.	6.6	52
609	Largeâ€Sized Ammonia Clusters and Solvation Energies of the Proton in Ammonia. Journal of Computational Chemistry, 2020, 41, 21-30.	1.5	30
610	The AQUAâ€MER databases and aqueous speciation server: A web resource for multiscale modeling of mercury speciation. Journal of Computational Chemistry, 2020, 41, 147-155.	1.5	3
611	Influence of Electrolyte Composition on Ultrafast Interfacial Electron Transfer in Fe-Sensitized TiO₂-Based Solar Cells. Journal of Physical Chemistry C, 2020, 124, 1794-1811.	1.5	19
612	On the mechanism of reduction of M(H₂O)_mⁿ⁺ by borohydride: the case of Ag(H₂O)₂⁺. Nanoscale, 2020, 12, 1657-1672.	2.8	13
613	Prediction of Alkanolamine pK_a Values by Combined Molecular Dynamics Free Energy Simulations and ab Initio Calculations. Journal of Chemical & Engineering Data, 2020, 65, 1358-1368.	1.0	6
614	Interplay between Ionization and Tautomerism in Bioactive Î²-Enamino Ester-Containing Cyclic Compounds: Study of Annulated 1,2,3,6-Tetrahydroazocine Derivatives. Journal of Physical Chemistry B, 2020, 124, 28-37.	1.2	3
615	Machine Learning-Guided Approach for Studying Solvation Environments. Journal of Chemical Theory and Computation, 2020, 16, 633-642.	2.3	52
616	The challenge of converting biomass polysaccharides into levulinic acid through heterogeneous catalytic processes. Biofuels, Bioproducts and Biorefining, 2020, 14, 417-445.	1.9	19
617	Unraveling the anti-influenza effect of flavonoids: Experimental validation of luteolin and its congeners as potent influenza endonuclease inhibitors. European Journal of Medicinal Chemistry, 2020, 208, 112754.	2.6	21
618	Method for the accurate prediction of electron transfer potentials using an effective absolute potential. Physical Chemistry Chemical Physics, 2020, 22, 25833-25840.	1.3	15
619	Solid acids, surface acidity and heterogeneous acid catalysis. Advances in Catalysis, 2020, 67, 1-90.	0.1	13
620	Absolute ion hydration free energy scale and the surface potential of water via quantum simulation. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 30151-30158.	3.3	14
621	Boosting Tunnel-Type Manganese Oxide Cathodes by Lithium Nitrate for Practical Aqueous Na-Ion Batteries. ACS Applied Energy Materials, 2020, 3, 10744-10751.	2.5	4
622	A polarizable molecular dynamics method for electrodeâ€“electrolyte interfacial electron transfer under the constant chemical-potential-difference condition on the electrode electrons. Journal of Chemical Physics, 2020, 153, 054126.	1.2	10

#	Article	IF	Citations
623	Thermodynamic and kinetic hydricity of transition metal hydrides. Chemical Society Reviews, 2020, 49, 7929-7948.	18.7	52
624	Experimental Validation of a Computational Screening Approach to Predict Redox Potentials for a Diverse Variety of Redox-Active Organic Molecules. Journal of Physical Chemistry C, 2020, 124, 24105-24114.	1.5	12
625	Computational studies of acidities of some hydroxycoumarins. Computational and Theoretical Chemistry, 2020, 1190, 113008.	1.1	3
626	Mechanistic Insights into the Conversion of Biorenewable Levoglucosanol to Dideoxysugars. ACS Sustainable Chemistry and Engineering, 2020, 8, 16339-16349.	3.2	4
627	An Extended Benchmark of Density Functionals for Calculating the Standard Reduction Potentials of Vanadium Compounds. Russian Journal of Physical Chemistry A, 2020, 94, 1616-1622.	0.1	2
628	Chlorinated Byproduct Formation during the Electrochemical Advanced Oxidation Process at MagnÃ©li Phase Ti₄O₇ Electrodes. Environmental Science & Technology, 2020, 54, 12673-12683.	4.6	49
629	An ABSINTH-Based Protocol for Predicting Binding Affinities between Proteins and Small Molecules. Journal of Chemical Information and Modeling, 2020, 60, 5188-5202.	2.5	5
630	A DFT study of the conformational and electronic properties of echinatin, a retrochalcone, and its anion in the gas phase and aqueous solution. Structural Chemistry, 2020, 31, 2513-2524.	1.0	12
631	Standard Values of the Thermodynamic Functions of the Formation of Ions in an Aqueous Solution and their Change during Solvation. Journal of Physical Chemistry A, 2020, 124, 11051-11060.	1.1	6
632	On the Spin-State Dependence of Redox Potentials of Spin Crossover Complexes. Inorganic Chemistry, 2020, 59, 18402-18406.	1.9	6
633	Destabilisation of gold cyanide complex by sulphur species: A computational perspective. Hydrometallurgy, 2020, 197, 105459.	1.8	4
634	From Synthetic to Biological Fe4S4Complexes: Redox Properties Correlated to Function of Radical Sâ€Adenosylmethionine Enzymes. ChemPlusChem, 2020, 85, 2534-2541.	1.3	3
635	Protonâ€“Electron Transfer to the Active Site Is Essential for the Reaction Mechanism of Soluble Î”⁹-Desaturase. Journal of the American Chemical Society, 2020, 142, 10412-10423.	6.6	24
636	Modeling temperature dependent and absolute carbamate stability constants of amines for CO2 capture. International Journal of Greenhouse Gas Control, 2020, 98, 103061.	2.3	10
637	Pushing the limits of the electrochemical window with pulse radiolysis in chloroform. Physical Chemistry Chemical Physics, 2020, 22, 14660-14670.	1.3	7
638	A computational study of the ground and excited state acidities of synthetic analogs of red wine pyranoanthocyanins. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	9
639	Surface pK_a of Saturated Carboxylic Acids at the Air/Water Interface: A Quantum Chemical Approach. Journal of Physical Chemistry C, 2020, 124, 13809-13818.	1.5	24
640	Hydrogenâ€“Deuterium Exchange in Basic Near-Critical and Supercritical Media: An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2020, 124, 2530-2536.	1.1	4

#	Article	IF	Citations
641	Computational Investigation into the Oxidation of Guanine to Form Imidazolone (Iz) and Related Degradation Products. Chemical Research in Toxicology, 2020, 33, 1010-1027.	1.7	5
642	Chemical Equilibrium of Zinc Acetate Complexes in Ethanol Solution. A Theoretical Description through Thermodynamic Cycles. Journal of Physical Chemistry B, 2020, 124, 3355-3370.	1.2	3
643	Effect of substitution on halide/hydrated halide binding: a case study of neutral bis-urea receptors. CrystEngComm, 2020, 22, 2197-2207.	1.3	7
644	Diferulate: A highly effective electron donor. Journal of Electroanalytical Chemistry, 2020, 869, 113950.	1.9	3
645	Electromechanics of the liquid water vapour interface. Physical Chemistry Chemical Physics, 2020, 22, 10676-10686.	1.3	14
646	The Role of the Organic Solvent Polarity in Isolating Uranyl Peroxide Capsule Fragments. Inorganic Chemistry, 2020, 59, 1633-1641.	1.9	11
647	The Case for Enzymatic Competitive Metal Affinity Methods. ACS Catalysis, 2020, 10, 2298-2307.	5.5	6
648	A blind SAMPL6 challenge: insight into the octanol-water partition coefficients of drug-like molecules via a DFT approach. Journal of Computer-Aided Molecular Design, 2020, 34, 463-470.	1.3	13
649	CO₂ Hydrogenation and Formic Acid Dehydrogenation Using Ir Catalysts with Amide-Based Ligands. Organometallics, 2020, 39, 1519-1531.	1.1	61
650	Cyclization step of noradrenaline and adrenaline autoxidation: a quantum chemical study. RSC Advances, 2020, 10, 16650-16658.	1.7	8
651	Synthesis and Properties of Sulfonated Copolymers of Oxadiazole, Dioxophenoxathiine, and Diphenyl Oxide. Polymer Science - Series B, 2020, 62, 47-60.	0.3	3
652	pKa values in the undergraduate curriculum: introducing pKa values measured in DMSO to illustrate solvent effects. ChemTexts, 2020, 6, 1.	1.0	11
653	Oxygen Atom Transfer as an Alternative Pathway for Oxygenâ€“Oxygen Bond Formation. Inorganic Chemistry, 2020, 59, 5966-5974.	1.9	12
654	A theoretical study on the pK_a values of selenium compounds in aqueous solution. New Journal of Chemistry, 2020, 44, 8325-8336.	1.4	4
655	Non-membrane solvent extraction desalination (SED) technology using solubility-switchable amine. Journal of Hazardous Materials, 2021, 403, 123636.	6.5	17
656	Computational insights into electrocatalytic CO2 reduction facilitated by Mn(I) half sandwich-based catalysts: Role of substitution and solvent. Electrochimica Acta, 2021, 366, 137463.	2.6	2
657	Determination of the absolute solvation free energy and enthalpy of the proton in solutions. Journal of Molecular Liquids, 2021, 322, 114919.	2.3	32
658	Interfacial microstructures and adsorption mechanisms of benzohydroxamic acid on Pb2+-activated cassiterite (1 1 0) surface. Applied Surface Science, 2021, 541, 148506.	3.1	12

#	Article	IF	Citations
659	How a Bismuth(III) Catalyst Achieves Greatest Activation of Organic Lewis Bases in a Catalytic Reaction: Insights from DFT Calculations. ChemCatChem, 2021, 13, 975-980.	1.8	5
660	Ambiguities in solvation free energies from cluster-continuum quasichemical theory: lithium cation in protic and aprotic solvents. Physical Chemistry Chemical Physics, 2021, 23, 16077-16088.	1.3	10
661	Electrocatalytic nitrate reduction with Co-based catalysts: comparison of DIM, TIM and cyclam ligands. Dalton Transactions, 2021, 50, 12324-12331.	1.6	8
662	Ab Initio Evaluation of the Redox Potential of Cytochrome c. Journal of Chemical Theory and Computation, 2021, 17, 1194-1207.	2.3	2
663	Nature of High- and Low-Affinity Metal Surface Sites on Birnessite Nanosheets. ACS Earth and Space Chemistry, 2021, 5, 66-76.	1.2	11
664	The pKa of Pentazole (HN5). Australian Journal of Chemistry, 2021, 74, 584.	0.5	4
665	Computational Investigation into the Mechanistic Features of Bromide-Catalyzed Alcohol Oxidation by PhIO in Water. Journal of Organic Chemistry, 2021, 86, 2998-3007.	1.7	3
666	Theoretical Determination of pKas of P(1)-H Phospholes and their Comparison with N(1)-H Azoles. Australian Journal of Chemistry, 2021, , .	0.5	2
667	From absolute potentials to a generalized computational standard hydrogen electrode for aqueous and non-aqueous solvents. Physical Chemistry Chemical Physics, 2021, 23, 11727-11737.	1.3	10
668	An amide-based second coordination sphere promotes the dimer pathway of Mn-catalyzed CO₂-to-CO reduction at low overpotential. Chemical Science, 2021, 12, 4779-4788.	3.7	19
669	Prediction Models on pK_a and Base-Catalyzed Hydrolysis Kinetics of Parabens: Experimental and Quantum Chemical Studies. Environmental Science & Technology, 2021, 55, 6022-6031.	4.6	31
670	Parameterization of Monovalent Ions for the OPC3, OPC, TIP3P-FB, and TIP4P-FB Water Models. Journal of Chemical Information and Modeling, 2021, 61, 869-880.	2.5	81
672	Ionic Liquid for PEDOT:PSS Treatment. Ion Binding Free Energy in Water Revealing the Importance of Anion Hydrophobicity. Journal of Physical Chemistry B, 2021, 125, 1916-1923.	1.2	25
673	Methane Generation from CO₂ with a Molecular Rhenium Catalyst. Inorganic Chemistry, 2021, 60, 3572-3584.	1.9	19
674	Condensed-phase relative Gibbs free energy and E/Z descriptors for 2-acetylthiophene and 2-acetylthiophene-N1-phenyl thiosemicarbazones. Journal of Molecular Modeling, 2021, 27, 101.	0.8	1
675	Dielectric continuum methods for quantum chemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1519.	6.2	91
676	On the NH and CH acidities of toluidine isomers: theoretical description and practical consequences for the synthesis of certain aniline dyes. Coloration Technology, 2021, 137, 389-398.	0.7	5
677	Theoretical investigation of the structural and electronic features of SLC-0111, a novel inhibitor of human carbonic anhydrase IX, and its anion. Structural Chemistry, 2021, 32, 1843-1856.	1.0	3

#	Article	IF	Citations
678	Computational Study of Intramolecular Coordination Enhanced Oxidative Addition to form PdIV-Pincer Complexes, and Selectivity in Aryloxide Attack at PdIVCH2CRRâ€² Motifs in Palladium-Mediated Organic Synthesis. Organometallics, 2021, 40, 1262-1269.	1.1	3
679	Equilibrium between triâ€•and tetraâ€coordinate chalcogenuranes is critical for cysteine protease inhibition. Journal of Computational Chemistry, 2021, 42, 1225-1235.	1.5	1
680	A simple method to calculate solution-phase free energies of charged species in computational electrocatalysis. Journal of Physics Condensed Matter, 2021, 33, 204001.	0.7	7
681	Distinct Mechanisms and Hydricities of Cp*Ir-Based CO₂ Hydrogenation Catalysts in Basic Water. ACS Catalysis, 2021, 11, 5776-5788.	5.5	17
682	Uncovering Differences in Hydration Free Energies and Structures for Model Compound Mimics of Charged Side Chains of Amino Acids. Journal of Physical Chemistry B, 2021, 125, 4148-4161.	1.2	41
683	Synthesis, Characterization, and Water Oxidation Activity of Isomeric Ru Complexes. Inorganic Chemistry, 2021, 60, 5791-5803.	1.9	16
684	Double-Carrousel Mechanism for Mn-Catalyzed Dehydrogenative Amide Synthesis from Alcohols and Amines. ACS Catalysis, 2021, 11, 6155-6161.	5.5	19
685	Mechanism of Ir-Mediated Selective Pyridine o-Câ€“H Activation: The Role of Lewis Acidic Boryl Group. ACS Catalysis, 2021, 11, 6186-6192.	5.5	7
686	Cooperativity and Anticooperativity in Ionâ€Water Interactions: Implications for the Aqueous Solvation of Ions. ChemPhysChem, 2021, 22, 1269-1285.	1.0	10
687	Enzymeâ€Inspired Design of Co II â€Based H 2 Generation Catalysts: A Toolbox with Guiding Principles Revealed by a Systematic DFT Study. European Journal of Inorganic Chemistry, 2021, 2021, 2739-2748.	1.0	0
688	Defluorodearomatization: A Photocatalytic Birch-Like Reduction That Enables Câ€“C Bond Formation and Provides Access to Unnatural Cannabinoids. Journal of Organic Chemistry, 2021, 86, 7928-7945.	1.7	7
689	Towards mild conditions by predictive catalysis via sterics in the Ru-catalyzed hydrogenation of thioesters. Molecular Catalysis, 2021, 510, 111692.	1.0	14
690	Titr-DMDâ€”A Rapid, Coarse-Grained Quasi-All-Atom Constant pH Molecular Dynamics Framework. Journal of Chemical Theory and Computation, 2021, 17, 4538-4549.	2.3	6
691	Reconciling the Experimental and Computational Hydrogen Evolution Activities of Pt(111) through DFT-Based Constrained MD Simulations. ACS Catalysis, 2021, 11, 8062-8078.	5.5	52
692	Kinetic Modeling of API Oxidation: (1) The AIBN/H₂O/CH₃OH Radical â€œSoupâ€• Molecular Pharmaceutics, 2021, 18, 3037-3049.	2.3	12
693	Advanced Materials for Energy-Water Systems: The Central Role of Water/Solid Interfaces in Adsorption, Reactivity, and Transport. Chemical Reviews, 2021, 121, 9450-9501.	23.0	43
694	Molecular-Level Insights into Selective Transport of Mg²⁺ in Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2021, 13, 51974-51987.	4.0	3
695	Proton-Coupled Group Transfer Enables Concerted Protonation Pathways Relevant to Small-Molecule Activation. Inorganic Chemistry, 2021, 60, 16953-16965.	1.9	8

#	Article	IF	Citations
696	Solvation free energy of the proton in acetonitrile. Journal of Molecular Liquids, 2021, 335, 116032.	2.3	21
697	Mechanistic Investigations into the Catalytic Levulinic Acid Hydrogenation, Insight in H/D Exchange Pathways, and a Synthetic Route to d₈-Î³-Valerolactone. ACS Catalysis, 2021, 11, 10467-10477.	5.5	15
698	Can hydrogen anion be a possible intermediate of the hydrogen electrode reaction?. Journal of Electroanalytical Chemistry, 2021, 896, 115150.	1.9	3
699	Using structure-function relationships to understand the mechanism of phenazine-mediated extracellular electron transfer in Escherichia coli. IScience, 2021, 24, 103033.	1.9	27
700	Computational study of bridgeâ€splitting, aryl halide oxidative addition to PtII, and reductive elimination from PtIV: a route to pincerâ€PtII reagents with chemical and biological applications. Chemistry - A European Journal, 2021, 27, 15426-15433.	1.7	0
701	How acid can become a dihydrogen complex in water? A DFT study. Journal of Organometallic Chemistry, 2021, 949, 121957.	0.8	3
702	Corrections in the CHARMM36 Parametrization of Chloride Interactions with Proteins, Lipids, and Alkali Cations, and Extension to Other Halide Anions. Journal of Chemical Theory and Computation, 2021, 17, 6240-6261.	2.3	7
703	DFT-Machine Learning Approach for Accurate Prediction of pK_a. Journal of Physical Chemistry A, 2021, 125, 8712-8722.	1.1	15
704	Esterification or Thioesterification of Carboxylic Acids with Alcohols or Thiols Using Amphipathic Monolith-SO3H Resin. Bulletin of the Chemical Society of Japan, 2021, 94, 2702-2710.	2.0	7
705	The antioxidant potential of retrochalcones isolated from liquorice root: A comparative DFT study. Phytochemistry, 2021, 192, 112964.	1.4	14
706	Insights into the role of hydroxyl group on carboxyl-modified MWCNTs in accelerating atenolol removal by Fe(III)/H2O2 system. Chemical Engineering Journal, 2021, 425, 130581.	6.6	25
707	Mechanism of iron complexes catalyzed in the N-formylation of amines with CO₂ and H₂: the superior performance of Nâ€“H ligand methylated complexes. Physical Chemistry Chemical Physics, 2021, 23, 16675-16689.	1.3	3
708	Cycloaddition mechanisms of CO₂ and epoxide catalyzed by salophen â€“ an organocatalyst free from metals and halides. Catalysis Science and Technology, 2021, 11, 2529-2539.	2.1	8
709	Iridium Complexes with Protonâ€Responsive Azoleâ€Type Ligands as Effective Catalysts for CO₂ Hydrogenation. ChemSusChem, 2017, 10, 4535-4543.	3.6	41
710	Balanced polarizable Drude force field parameters for molecular anions: phosphates, sulfates, sulfamates, and oxides. Journal of Molecular Modeling, 2020, 26, 152.	0.8	12
711	On the Accuracy of the Direct Method to Calculate pK_a from Electronic Structure Calculations. Journal of Physical Chemistry A, 2021, 125, 65-73.	1.1	39
712	Molecular Oxygen Activation at a Conducting Polymer: Electrochemical Oxygen Reduction Reaction at PEDOT Revisited, a Theoretical Study. Journal of Physical Chemistry C, 2020, 124, 13263-13272.	1.5	32
713	A pentadentate nitrogen-rich copper electrocatalyst for water reduction with pH-dependent molecular mechanisms. Dalton Transactions, 2017, 46, 16812-16820.	1.6	21

#	Article	IF	Citations
714	G4 accuracy at DFT cost: unlocking accurate redox potentials for organic molecules using systematic error cancellation. Physical Chemistry Chemical Physics, 2020, 22, 4439-4452.	1.3	13
715	Solvation energies of ions with ensemble cluster-continuum approach. Physical Chemistry Chemical Physics, 2020, 22, 22357-22368.	1.3	28
716	Does addition of 1-octanol as a phase modifier provide radical scavenging radioprotection for N,N,Nâ€²,Nâ€²-tetraoctyldiglycolamide (TODGA)?. Physical Chemistry Chemical Physics, 2020, 22, 24978-24985.	1.3	12
717	Measuring Absolute Single Half-Cell Reduction Potentials with Mass Spectrometry. Electroanalytical Chemistry, A Series of Advances, 2013, , 1-32.	1.7	1
718	Molecular Perspective Review of Biochemical Role of Nucleobases Modified by Oxidative Stress. Computational Methods in Science and Technology, 2010, 16, 51-72.	0.3	5
719	With or without light: comparing the reaction mechanism of dark-operative protochlorophyllide oxidoreductase with the energetic requirements of the light-dependent protochlorophyllide oxidoreductase. PeerJ, 2014, 2, e551.	0.9	5
720	Influence of uranyl complexation on the reaction kinetics of the dodecane radical cation with used nuclear fuel extraction ligands (TBP, DEHBA, and DEHiBA). Physical Chemistry Chemical Physics, 2021, 23, 24589-24597.	1.3	13
721	Charge neutral halogen bonding tetradentate-iodotriazole macrocycles capable of anion recognition and sensing in highly competitive aqueous media. Chemical Communications, 2021, 57, 11976-11979.	2.2	9
722	Improving the study of proton transfers between amino acid side chains in solution: choosing appropriate DFT functionals and avoiding hidden pitfalls. Highlights in Theoretical Chemistry, 2013, , 199-205.	0.0	0
723	Nitrogen Acids. , 2013, , 77-92.		0
724	Comprehensive Comparative Study Using Ab Initio Computational Approaches on the Structures of Cisplatin, Oxaliplatin and BNP3029 (A Novel Substituted Cyano Ligand-based Platinum Analogue) and Activation Energy Barriers for the Attack of Nucleophiles on Cisplatin and BNP3029 and their Monoaquated Derivatives. , 2014, 4, .		1
725	Thermodynamic Parameters for Solvation of Nano ZNO and Its Dopes In 50% DMSO - 50% DMF (V/V) Solutions at Different Temperatures. Energy Review, 2014, 1, 44-55.	0.0	0
726	SÃure-Base-Gleichgewichte. , 2018, , 17-93.		0
728	Density Functional Theory Study on the Initial Reactions of D-Xylose and D-Xylulose Dehydration to Furfural. Carbohydrate Research, 2021, 511, 108463.	1.1	6
729	Interphase interactions of hydrophobic powders based on methilsilica in the water environment. Surface, 2020, 12(27), 53-99.	0.4	0
730	Enhanced Synthesis of oxo-Verdazyl Radicals Bearing Sterically-and Electronically-Diverse C3-Substitents. Organic and Biomolecular Chemistry, 2021, 19, 10120-10138.	1.5	6
731	Adhesion of Colloids and Bacteria to Porous Media: A Critical Review. Reviews of Adhesion and Adhesives, 2019, 7, 417-460.	3.3	1
732	Quantum Calculations of pKa values for Some Amine Compounds. , 2020, , .		0

#	Article	IF	Citations
733	Theoretical Study of the Microhydration the Chemical Warfare Agent Sulfur Mustard. ACS Omega, 2020, 5, 1822-1831.	1.6	1
734	Density Functional Theory Calculations of Redox Potentials of Neptunium Complexes in Ionic Liquid. Journal of the Electrochemical Society, 2020, 167, 136503.	1.3	3
735	Single-ion solvation free energy: A new clusterâ€“continuum approach based on the cluster expansion method. Physical Chemistry Chemical Physics, 2021, 23, 26902-26910.	1.3	9
736	Visible light-driven carbon-carbon reductive coupling of aromatic ketones activated by Ni-doped CdS quantum dots: An insight into the mechanism. Applied Catalysis B: Environmental, 2022, 304, 120946.	10.8	15
737	Platinum(<scp>II</scp>)â€mediated disulfide/thiolate interconversion in organic disulfides: <scp>Density functional theory</scp> thermodynamic study. International Journal of Quantum Chemistry, 2022, 122, e26849.	1.0	2
738	Photochemical conversion of CO₂ to CO by a Re complex: theoretical insights into the formation of CO and HCO₃^{â˜} from an experimentally detected monoalkyl carbonate complex. RSC Advances, 2021, 11, 37713-37725.	1.7	6
739	Fourier Transform Infrared Spectroscopy and Vibrational Circular Dichroism Assisted Elucidation of the Solution-State Supramolecular Speciation in Racemic and Enantiopure Ketoprofen. Applied Spectroscopy, 2022, , 000370282110600.	1.2	1
740	Role of Bimetallic Interactions in the Enhancement of Catalytic CO₂ Reduction by a Macrocyclic Cobalt Catalyst. ACS Catalysis, 2022, 12, 1706-1717.	5.5	15
741	How are transition states modeled in heterogeneous electrocatalysis?. Current Opinion in Electrochemistry, 2022, 33, 100940.	2.5	20
742	Reply to the â€œComment on â€˜On the Accuracy of the Direct Method to Calculate pK_a from Electronic Structure Calculationsâ€™â€• Journal of Physical Chemistry A, 2022, 126, 650-651.	1.1	1
743	Comment on â€œOn the Accuracy of the Direct Method to Calculate pKa from Electronic Structure Calculationsâ€• Journal of Physical Chemistry A, 2022, 126, 648-649.	1.1	1
744	Two-Stage Catalysis in the Pd-Catalyzed Formation of 2,2,2-Trifluoroethyl-Substituted Acrylamides: Oxidative Alkylation of PdII by an IIII Reagent and Roles for Acetate, Triflate, and Triflic Acid. Organometallics, 0, , .	1.1	4
745	Acid Dissociation Constants of the Benzimidazole Unit in the Polybenzimidazole Chain: Configuration Effects. Molecules, 2022, 27, 1064.	1.7	1
746	Calculations of pK_a Values for a Series of Naturally Occurring Modified Nucleobases. Journal of Physical Chemistry A, 2022, 126, 1518-1529.	1.1	16
747	Accelerating Solvent Selection for Type II Porous Liquids. Journal of the American Chemical Society, 2022, 144, 4071-4079.	6.6	11
748	Ionization Energies and Redox Potentials of Hydrated Transition Metal Ions: Evaluation of Domain-Based Local Pair Natural Orbital Coupled Cluster Approaches. Journal of Chemical Theory and Computation, 2022, 18, 1619-1632.	2.3	9
749	A Bidirectional Bioinspired [FeFe]-Hydrogenase Model. Journal of the American Chemical Society, 2022, 144, 3614-3625.	6.6	31
750	Theoretical Modeling of Electrochemical Proton-Coupled Electron Transfer. Chemical Reviews, 2022, 122, 10599-10650.	23.0	83

#	Article	IF	Citations
751	Metal-ligand bonding in bispidine chelate complexes for radiopharmaceutical applications. Structural Chemistry, 2023, 34, 5-15.	1.0	3
752	Design strategies for low temperature aqueous electrolytes. , 2022, 1, e9120003.		94
753	Optimal temperature for the absorption of C₂-C₅ mercaptans by sodium hydroxide solutions from isooctane. Petroleum Science and Technology, 0, , 1-13.	0.7	0
754	Predictive energetic tuning of C-Nucleophiles for the electrochemical capture of carbon dioxide. IScience, 2022, 25, 103997.	1.9	4
755	Electron-induced fragmentation of water droplets: Simulation study. Journal of Chemical Physics, 2022, 156, 144303.	1.2	1
756	DFT investigation on the carbonate radical formation in the system containing carbon dioxide and hydroxyl free radical. Journal of Molecular Graphics and Modelling, 2022, 114, 108182.	1.3	3
757	Implicit Solvation Methods for Catalysis at Electrified Interfaces. Chemical Reviews, 2022, 122, 10777-10820.	23.0	82
758	Rational Design of Nonbonded Point Charge Models for Monovalent Ions with Lennard-Jones 12â€“6 Potential. Journal of Physical Chemistry B, 2021, 125, 13502-13518.	1.2	10
759	Benchmark Study of Redox Potential Calculations for Ironâ€“Sulfur Clusters in Proteins. Inorganic Chemistry, 2022, 61, 5991-6007.	1.9	8
760	Theoretical study of heptadentate bispidine ligands for radiopharmaceutic applications. Computational and Theoretical Chemistry, 2022, 1212, 113716.	1.1	1
762	Automated Molecular Cluster Growing for Explicit Solvation by Efficient Force Field and Tight Binding Methods. Journal of Chemical Theory and Computation, 2022, 18, 3174-3189.	2.3	45
763	Salt-Enhanced Oxidative Addition of Iodobenzene to Pd: An Interplay Between Cation, Anion, and Pdâ€“Pd Cooperative Effects. Inorganic Chemistry, 2022, 61, 7935-7944.	1.9	6
764	How to Predict the pK_a of Any Compound in Any Solvent. ACS Omega, 2022, 7, 17369-17383.	1.6	20
765	Computational study of BrÃ¸nsted acidity in the metalâ€“organic framework UiO-66. Chemical Physics Letters, 2022, 800, 139658.	1.2	2
766	Computational comparison of Ru(bda)(py)₂ and Fe(bda)(py)₂ as water oxidation catalysts. Dalton Transactions, 2022, 51, 8618-8624.	1.6	1
767	Mechanistic Insights into Cobalt-Based Water Oxidation Catalysis by DFT-Based Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2022, 126, 3301-3310.	1.1	5
768	A Non-Bornian Approach to the Standard Gibbs Energy of Ion Transfer at the Oil | Water Interface. Review of Polarography, 2022, 68, 3-14.	0.0	0
769	Self-Assembled Liposomes Enhance Electron Transfer for Efficient Photocatalytic CO₂ Reduction. Journal of the American Chemical Society, 2022, 144, 9399-9412.	6.6	23

#	Article	IF	Citations
770	Structures, temperature effect, binding and clustering energies of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si124.svg"><mml:mrow><mml:msup><mml:mrow><mml:mi mathvariant="normal">Cu</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup><mml:mo stretchy="false">(</mml:mo><mml:mi mathvariant="normal">MeOH</mml:mi><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 722 Td	2.3	4
771	DFT characterisation of a Pd^{II} â† I^{III} adduct, and a Pd^{II} complex formed after oxidative alkenylation of Pd^{II} by [Ph(alkenyl)I^{III}]⁺, in Pd-mediated synthesis of benzofurans involving Pd^{IV}, annulation and chain-walking. Dalton Transactions, 2022, 51, 9377-9384.	1.6	3
772	Geometrical benchmarking and analysis of redox potentials of copper(I/<scp>II</scp>) <scp>guanidineâ€quinoline</scp> complexes: Comparison of semiâ€empirical tightâ€binding and <scp>DFT</scp> methods and the challenge of describing the entatic state (part <scp>III</scp>). Journal of Computational Chemistry, 2023, 44, 319-328.	1.5	1
773	The mechanisms and molecular properties about isomerization of resin acids, synthesis of acrylopimaric acid based on DFT Calculation. Journal of Physical Organic Chemistry, 0, , .	0.9	0
774	Theoretical Study of The Role of the Non-innocent Phenolate Ligand of a Nickel Complex in Water Oxidation. Physical Chemistry Chemical Physics, 0, , .	1.3	0
775	Impacts of targeting different hydration free energy references in the development of ion potentials. Physical Chemistry Chemical Physics, 0, , .	1.3	0
777	Kinetics and mechanism of the reaction of hydrogen peroxide with hypochlorous acid: Implication on electrochemical water treatment. Journal of Hazardous Materials, 2022, 438, 129420.	6.5	7
778	Engineering of iridium complexes for the efficient hydrogen evolution of formic acid without additives. Journal of Catalysis, 2022, 413, 119-126.	3.1	6
779	Photocatalytic CO2 reduction by a Z-scheme mechanism in an aqueous suspension of particulate (CuGa)0.3Zn1.4S2, BiVO4 and a Co complex operating dual-functionally as an electron mediator and as a cocatalyst. Applied Catalysis B: Environmental, 2022, 316, 121600.	10.8	8
780	Non-Heme Oxoiron complexes as active intermediates in water oxidation process with hydrogen/oxygen atom transfer reactions. Dalton Transactions, 0, , .	1.6	0
781	Computation of Oxidation Potentials of Solvated Nucleobases by Static and Dynamic Multilayer Approaches. Journal of Chemical Information and Modeling, 2022, 62, 3365-3380.	2.5	5
782	Density Functional Theory Modeling of the Oxidation Mechanism of Co(II) by Birnessite. ACS Earth and Space Chemistry, 2022, 6, 2063-2075.	1.2	6
783	Determination of Sulfite Content in Wet FGD Slurry by Noâ€Acidâ€Additive Iodimetry: Experimental and DFT Studies. ChemistrySelect, 2022, 7, .	0.7	0
784	Challenges in predicting Î”rxnG in solution: The chelate effect. Journal of Chemical Physics, 2022, 157, .	1.2	1
785	Density Functional Study on the Deprotonation and Binding Mechanism of Imidazole on Gold Electrodes in an Aqueous Environment. Journal of Physical Chemistry C, 2022, 126, 12424-12434.	1.5	1
786	Molecular dynamics insight into phase separation and transport in anion-exchange membranes: Effect of hydrophobicity of backbones. Journal of Membrane Science, 2022, 661, 120922.	4.1	28
787	Closed Aromatic TubesÂâ€ÂCapsularenes. Angewandte Chemie, 0, , .	1.6	0
788	Theoretical Relations between Electronic and Ionic Work Functions, Standard Reduction Potentials for Metal Dissolution and the Corrosion Potential. Journal of the Electrochemical Society, 2022, 169, 081506.	1.3	3

#	Article	IF	Citations
789	Closed Aromatic TubesÂâ€ÂCapsularenes. Angewandte Chemie - International Edition, 0, , .	7.2	2
790	Aqueous Speciation of Tetravalent Actinides in the Presence of Chloride and Nitrate Ligands. Inorganic Chemistry, 2022, 61, 14718-14725.	1.9	4
791	Probing Nanoconfined Ion Transport in Electrified 2D Laminate Membranes with Electrochemical Impedance Spectroscopy. Small Methods, 2022, 6, .	4.6	3
792	Hydrogen Bond Thermodynamics in Aqueous Acid Solutions: A Combined DFT and Classical Force-Field Approach. Journal of Physical Chemistry A, 2022, 126, 7382-7398.	1.1	5
793	Predicting Solvent Effects on S_N2 Reaction Rates: Comparison of QM/MM, Implicit, and MM Explicit Solvent Models. Journal of Physical Chemistry B, 2022, 126, 9047-9058.	1.2	9
794	In silico designing of Si- and Ge-doped imidazolium: a new heterocyclic aromatic superacid. Theoretical Chemistry Accounts, 2022, 141, .	0.5	0
795	Ion Solvation Free Energy Calculation Based on Ab Initio Molecular Dynamics Using a Hybrid Solvent Model. Journal of Chemical Theory and Computation, 2022, 18, 6878-6891.	2.3	4
796	The multiple roles of phenols in the degradation of aniline contaminants by sulfate radicals: A combined study of DFT calculations and experiments. Journal of Hazardous Materials, 2023, 443, 130216.	6.5	4
797	Synthesis, characterization, theoretical studies and antioxidant and cytotoxic evaluation of a series of Tetrahydrocurcumin (THC)-benzylated derivatives. Journal of Molecular Structure, 2023, 1273, 134355.	1.8	2
798	Group 6 (Cr, Mo, W) and Group 7 (Mn, Re) bipyridyl tetracarbonyl complex for electrochemical CO2 conversion: DFT and DLPNO-CCSD(T) study for effects of the central metal on redox potential, thermodynamics, and kinetics. Chemical Physics, 2023, 565, 111758.	0.9	2
799	Electronic Substitution Effect on the Ground and Excited State Properties of Indole Chromophore: A Computational Study**. ChemPhysChem, 2023, 24, .	1.0	3
800	Unraveling the Electrochemistry of Verdazyl Species in Acidic Electrolytes for the Application in Redox Flow Batteries. Chemistry of Materials, 2022, 34, 10424-10434.	3.2	4
801	A benzo[a]phenazine-based redox species with highly reversible two-electron reaction for aqueous organic redox flow batteries. Electrochimica Acta, 2023, 439, 141644.	2.6	5
802	Host-guest complexation of cucurbit[7]uril and cucurbit[8]uril with the antimuscarinic drugs tropicamide and atropine. Journal of Molecular Graphics and Modelling, 2023, 119, 108380.	1.3	4
803	Quantum Mechanical Calculations of Redox Potentials of the Metal Clusters in Nitrogenase. Molecules, 2023, 28, 65.	1.7	2
804	Biological activity of mixed chelate copper(II) complexes, with substituted diimine and tridentate Schiff bases (NNO) and their hydrogenated derivatives as secondary ligands: CasiopeÃna's fourth generation. Journal of Inorganic Biochemistry, 2023, 242, 112097.	1.5	9
805	<scp>MoBioTools</scp> : A toolkit to setup quantum mechanics/molecular mechanics calculations. Journal of Computational Chemistry, 0, , .	1.5	7
806	Effects of ancillary ligands in acceptorless benzyl alcohol dehydrogenation mediated by phosphine-free cobalt complexes. Frontiers of Chemical Science and Engineering, 0, , .	2.3	1

#	Article	IF	Citations
807	Absolute Hydration Free Energy of Small Anions and the Aqueous pK_a of Simple Acids. Journal of Physical Chemistry A, 2022, 126, 9190-9206.	1.1	1
808	Effects of nitrate and Fe/As molar ratio on direct iron(III)-arsenite precipitation in high-sulfateâ€“chloride wastewaters. Environmental Science and Pollution Research, 0, , .	2.7	0
809	Benchmarking the computed proton solvation energy and absolute potential in non-aqueous solvents. Electrochimica Acta, 2023, 443, 141785.	2.6	2
810	Redox Potentials with COSMO-RS: Systematic Benchmarking with Different Databases. Journal of Chemical Theory and Computation, 2023, 19, 1014-1022.	2.3	7
811	Solvation of Manganese(III) Ion in Water and in Ammonia. Journal of Physical Chemistry A, 2023, 127, 1103-1111.	1.1	3
812	Systematic Theoretical Study on the pH-Dependent Absorption and Fluorescence Spectra of Flavins. Molecules, 2023, 28, 3315.	1.7	0
813	A bioinspired cobalt catalyst based on a tripodal imidazole/pyridine platform capable of water reduction and oxidation. Journal of Inorganic Biochemistry, 2023, 242, 112162.	1.5	0
814	Further reflections about the â€œBornâ€•term used in thermodynamic models for electrolytes. Journal of Molecular Liquids, 2023, 380, 121713.	2.3	3
815	Software Able to Assist Electrochemistry. , 2011, , 110-152.		0
816	An Efficient Multilayer Approach to Model DNA-Based Nanobiosensors. Journal of Physical Chemistry B, 2023, 127, 1513-1525.	1.2	0
817	How Protons Move in Enzymesâ”€The Case of Nitrogenase. Journal of Physical Chemistry B, 2023, 127, 2156-2159.	1.2	4
818	Impact of ethylene glycol on ions influencing corrosion in pores between iron oxide and calcium carbonate. Molecular Simulation, 2023, 49, 664-677.	0.9	0
819	Structure, Properties, and Reactivity of Polyoxocationic Zirconium and Hafnium Clusters: A Computational Investigation. Inorganic Chemistry, 2023, 62, 5081-5087.	1.9	2
820	Calculated pK_a Values for a Series of Aza- and Deaza-Modified Nucleobases. Journal of Physical Chemistry A, 2023, 127, 3526-3534.	1.1	2
821	Reactivity Factors in Catalytic Methanogenesis and Their Tuning upon Coenzyme F430 Biosynthesis. Journal of the American Chemical Society, 2023, 145, 9039-9051.	6.6	1