Yu-Xiang Bu

List of Publications by Year
in descending order

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215 papers	2,455 citations	304743 22 h-index	361022 35 g-index
216 all docs	216 docs citations	216 times ranked	2164 citing authors

#	Article	IF	Citations
1	Interplay between invasive single atom Pt and native oxygen vacancy in rutile TiO2(110) surface: A theoretical study. Nano Research, 2022, 15, 669-676.	10.4	15
2	Organic ligand mediated evolution from aluminum-based superalkalis to superatomic molecules and one-dimensional nanowires. Nano Research, 2022, 15, 1162-1170.	10.4	11
3	Intriguing strain-governed magnetic phase transitions in 2D vanadium porphyrin sheets. Physical Chemistry Chemical Physics, 2022, 24, 3834-3843.	2.8	2
4	Unique Solvated Electron State and Its Remarkable Enhancement Effect on Internuclear J-Couplings in Fluorocarbon Cage Electron Clathrates. Journal of Physical Chemistry C, 2022, 126, 4965-4974.	3.1	3
5	Dual External Field-Engineered Hyperhalogen. Journal of Physical Chemistry Letters, 2022, 13, 3942-3948.	4.6	4
6	Endohedral Ï*f*-Diradical Nitrogen-Vacancy Diamond Nanoclusters with a Confined Magnetic Space and Strong Electronic Spin Couplings. Journal of Physical Chemistry A, 2022, 126, 3174-3184.	2.5	3
7	Modulation of proton-coupled electron transfer reactions in lysine-containing alpha-helixes: alpha-helixes promoting long-range electron transfer. Physical Chemistry Chemical Physics, 2022, 24, 14592-14602.	2.8	2
8	Magnetic couplings and applied electric field regulation in diradical SiC defect diamond-like nanoclusters. New Journal of Chemistry, 2022, 46, 14676-14689.	2.8	1
9	Functionalization of [60]Fullerene through photochemical reaction for fulleropyrrolidine nanovectors synthesis: Experimental and theoretical approaches. Colloids and Surfaces B: Biointerfaces, 2021, 198, 111457.	5.0	1
10	TD-DFT Studies on sp- and sp²-Hybridized Single Vacancy-Defected [60]Fullerene: Electronic Excitation and Nonlinear Optical Properties of C59 [9-4] and C59 [8-5] Isomers. Journal of Physical Chemistry A, 2021, 125, 106-114.	2.5	10
11	A facile strategy for synthesis of porous Cu₂O nanospheres and application as nanozymes in colorimetric biosensing. Journal of Materials Chemistry B, 2021, 9, 3533-3543.	5.8	23
12	Electric field controlled uphill electron migration along Î±-helical oligopeptides. Physical Chemistry Chemical Physics, 2021, 23, 1464-1474.	2.8	2
13	Regulating Work Function of [Ca24Al28O64]4+:4eâ€“ Electrides Via Changing Solvated Electron Characters. Journal of Physical Chemistry Letters, 2021, 12, 3274-3280.	4.6	5
14	Dual-atom Pt heterogeneous catalyst with excellent catalytic performances for the selective hydrogenation and epoxidation. Nature Communications, 2021, 12, 3181.	12.8	156
15	Regulating the Catalytic Performance of a Dual-Atom Iron Species Deposited on Graphitic Carbon Nitride for Electrochemical Nitrogen Reduction. Journal of Physical Chemistry C, 2021, 125, 14253-14262.	3.1	18
16	Observation of â€œOutlawâ€•Dual Aromaticity in Unexpectedly Stable Open-Shell Metal Clusters Caused by Near-Degenerate Molecular Orbital Coupling. CCS Chemistry, 2021, 3, 1913-1920.	7.8	2
17	Molecular Dynamics Characterization of Dielectron Hydration in Liquid Water with Unique Double Proton Transfers. Journal of Chemical Theory and Computation, 2021, 17, 666-677.	5.3	7
18	A sandwich-like Ga₂FeS₄-supported single metal atom as a promising bifunctional electrocatalyst for overall water splitting. Journal of Materials Chemistry A, 2021, 9, 18594-18603.	10.3	4

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19	Adsorption energy as a promising single-parameter descriptor for single atom catalysis in the oxygen evolution reaction. Journal of Materials Chemistry A, 2021, 9, 6442-6450.	10.3	18
20	Molecular dynamics insights into electron-catalyzed dissociation repair of cyclobutane pyrimidine dimer. Chinese Journal of Chemical Physics, 2021, 34, 850-860.	1.3	0
21	Hydroxide-Enhanced Superexchange Magnetic Couplings in Ionic Clathrate Hydrates. Journal of Physical Chemistry C, 2020, 124, 25455-25464.	3.1	0
22	Azomethine ylide addition impact on functionalized [60]Fullerene and [60]Boron-Nitride: Anticancer Doxorubicin and Boronic Chalcone drugs binding characteristics with mono- and bis-nanocarriers. Colloids and Surfaces B: Biointerfaces, 2020, 196, 111277.	5.0	7
23	General Dual-Switched Dynamic Singlet Fission Channels in Solvents Governed Jointly by Chromophore Structural Dynamics and Solvent Impact: Singlet Prefission Energetics Analyses. Journal of the American Chemical Society, 2020, 142, 17469-17479.	13.7	14
24	Intriguing Radicalâ€“Radical Interactions in Doubly Reduced Dimers: Cytosine Anion Radical versus Hydrogenated Cytosine Radical. Journal of Physical Chemistry C, 2020, 124, 19760-19773.	3.1	1
25	Spatial Confinement as an Effective Strategy for Improving the Catalytic Selectivity in Acetylene Hydrogenation. ACS Applied Materials & Interfaces, 2020, 12, 39352-39361.	8.0	11
26	Surface Modification Strategy for Promoting the Performance of Non-noble Metal Single-Atom Catalysts in Low-Temperature CO Oxidation. ACS Applied Materials & Interfaces, 2020, 12, 19457-19466.	8.0	12
27	Tuning the Electronic Properties and Performance of Low-Temperature CO Oxidation of the Gold Cluster by Oriented External Electronic Field. Journal of Physical Chemistry Letters, 2020, 11, 1093-1099.	4.6	23
28	Magnetic Dioxygen Clathrate Hydrates: A Type of Promising Building Blocks for Icy Crystalline Materials. Journal of Physical Chemistry C, 2020, 124, 10669-10678.	3.1	4
29	Rational design of an efficient descriptor for single-atom catalysts in the hydrogen evolution reaction. Journal of Materials Chemistry A, 2020, 8, 9202-9208.	10.3	41
30	Effect of Paramagnetic Open-Shell Gadolinium(III) Texaphyrin on Its Kinetics and Electronic Structures in Fluorescence and Phosphorescence Emission States. Journal of Physical Chemistry C, 2019, 123, 28327-28335.	3.1	6
31	Rational magnetic modification of N,N-dioxidized pyrazine ring expanded adenine and thymine: a diradical character induced by base pairing and double protonation. Physical Chemistry Chemical Physics, 2019, 21, 20095-20106.	2.8	3
32	Unexpected diradical character and large magnetic spin coupling in modified porphyrins induced by inverting pyrrole rings. Physical Chemistry Chemical Physics, 2019, 21, 17209-17220.	2.8	8
33	A green and general strategy for the synthesis of hollow Ag/CdS nanocomposites for superior SERS performance. CrystEngComm, 2019, 21, 3709-3720.	2.6	7
34	Rational Design of Organic Magnets with Switchable Two-Way Couplers: Magnetic Modulation or Switching through Lactamâ€“Lactim Tautomerization. Journal of Physical Chemistry C, 2019, 123, 14152-14163.	3.1	4
35	Proton-Transfer-Regulated Magnetic Spin Couplings in Nitroxide-Functionalized Porphycene Diradicaloids. Journal of Physical Chemistry C, 2019, 123, 10764-10776.	3.1	7
36	Nonlinear Migration Dynamics of Excess Electrons along Linear Oligopeptides Controlled by an Applied Electric Field. ChemPhysChem, 2019, 20, 1497-1507.	2.1	2

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37	Intriguing electric field effect on magnetic spin couplings in dielectron clathrate hydrates. International Journal of Quantum Chemistry, 2019, 119, e25916.	2.0	4
38	Polymeric tungsten carbide nanoclusters: structural evolution, ligand modulation, and assembled nanomaterials. Nanoscale, 2019, 11, 19903-19911.	5.6	20
39	Dynamic relaying properties of a Î²â€turn peptide in longâ€range electron transfer. Journal of Computational Chemistry, 2019, 40, 988-996.	3.3	3
40	Dynamics Insight into Isomerization and Dissociation of Hot Criegee Intermediate CH3CHOO. Journal of Physical Chemistry A, 2019, 123, 1085-1090.	2.5	18
41	Azobenzeneâ€bridged diradical janus nucleobases with photoâ€converted magnetic properties between antiferromagnetic and ferromagnetic couplings. Journal of Computational Chemistry, 2018, 39, 1398-1405.	3.3	3
42	Spin coupling interactions in Cî€€ or Bâ€“B-cored porphyrin-mimetic graphene patch nitroxide diradicals. Physical Chemistry Chemical Physics, 2018, 20, 8099-8111.	2.8	4
43	Unusual Indirect Nuclear Spinâ€“Spin Exchange Coupling through Solvated Electron. Journal of Physical Chemistry Letters, 2018, 9, 689-695.	4.6	10
44	Remarkable Differences in Spin Couplings for Various Selfâ€Paired Dimers of Ringâ€Expansionâ€Radicalized Uracil: Aâ€‰Basis for the Design of Magnetically Anisotropic Assemblies. ChemPhysChem, 2018, 19, 208-219.	2.1	5
45	Dielectron Clathrate Hydrates with Unique Superexchange Spin Couplings. Journal of Physical Chemistry C, 2018, 122, 7635-7641.	3.1	4
46	Unique Solvating Effect in Azabenzene Clathrate Hydrates. Journal of Physical Chemistry C, 2018, 122, 28466-28477.	3.1	1
47	Rational Design of Magnetic DNA Motifs with Diradical Character: Nitroxide Functionalization of Nucleobases. Journal of Physical Chemistry C, 2018, 122, 16488-16497.	3.1	4
48	Intriguing diaza effects on magnetic coupling characteristics in diazaâ€benzo[k]tetrapheneâ€bridged nitroxide diradicals. International Journal of Quantum Chemistry, 2018, 118, e25693.	2.0	4
49	Computational design of three Cu-induced triangular pyrimidines based DNA motifs with improved conductivity. Canadian Journal of Chemistry, 2017, 95, 571-579.	1.1	0
50	First principles investigation of the mechanical, thermodynamic and electronic properties of FeSn5 and CoSn5 intermetallic phases under pressure. Journal of the Korean Physical Society, 2017, 70, 375-381.	0.7	4
51	Diradicalized biphenyl derivative carbon-based material molecules: exploring the tuning effects on magnetic couplings. Physical Chemistry Chemical Physics, 2017, 19, 5932-5943.	2.8	12
52	Regio- and Diastereoselective Cross-Dehydrogenative Coupling of Tetrahydropyridines with 1,3-Dicarbonyl Compounds. Organic Letters, 2017, 19, 2146-2149.	4.6	27
53	Protonation-modulated localization of excess electrons in histidine aqueous solutions revealed by ab initio molecular dynamics simulations: anion-centered versus cation-centered localization. Physical Chemistry Chemical Physics, 2017, 19, 13807-13818.	2.8	3
54	Remarkable Magnetic Coupling Interactions in Multi-Beryllium-Expanded Small Graphene-like Molecules with Well-Defined Polyradical Characters. Organometallics, 2017, 36, 1505-1514.	2.3	4

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55	Facile and economical synthesis of ZnS nanotubes and their superior adsorption performance for organic dyes. CrystEngComm, 2017, 19, 2380-2393.	2.6	36
56	Cu-wire-mediatedÂdipyrimidineÂbaseÂpairsÂasÂthe buildingÂblocksÂforÂ conductive and magnetic Cuâ€“DNAÂ nanowires. Journal of Mathematical Chemistry, 2017, 55, 1301-1321.	1.5	3
57	Efficient floating diffuse functions for accurate characterization of the surface-bound excess electrons in water cluster anions. Physical Chemistry Chemical Physics, 2017, 19, 2816-2825.	2.8	3
58	Core-Modified Porphyrin Diradicals with a Câ•C Unit: Redox-Driven Magnetic Switching. Journal of Physical Chemistry C, 2017, 121, 21231-21243.	3.1	16
59	Tuning the Spin Coupling Interactions in the Nitroxideâ€Based Bisphenolâ€Like Diradicals. ChemPhysChem, 2017, 18, 2487-2498.	2.1	9
60	Protonation-Enhanced Antiferromagnetic Couplings in Azobenzene-Bridged Diradicals. Journal of Physical Chemistry C, 2017, 121, 17160-17168.	3.1	17
61	Reduced graphene oxide-stabilized copper nanocrystals with enhanced catalytic activity and SERS properties. RSC Advances, 2016, 6, 50587-50594.	3.6	20
62	Computational insights into intriguing vibration-induced pulsing diradical character in perfluoropentacene and the perfluorination effect. Physical Chemistry Chemical Physics, 2016, 18, 16179-16187.	2.8	3
63	Mechanisms Responsible for High Energy Radiation Induced Damage to Single-Stranded DNA Modified by Radiosensitizing 5-Halogenated Deoxyuridines. Journal of Physical Chemistry B, 2016, 120, 2649-2657.	2.6	12
64	Molecular Vibrations Induced Potential Diradical Character in Hexazapentacene. Journal of Physical Chemistry C, 2016, 120, 10215-10226.	3.1	11
65	Bifurcate localization modes of excess electron in aqueous Ca²⁺â¯amide solution revealed by ab initio molecular dynamics simulation: towards hydrated electron versus hydrated amide anion. Physical Chemistry Chemical Physics, 2016, 18, 18868-18879.	2.8	2
66	Benchmark calculations of excess electrons in water cluster cavities: balancing the addition of atom-centered diffuse functions versus floating diffuse functions. Physical Chemistry Chemical Physics, 2016, 18, 23812-23821.	2.8	5
67	The Equally Important Role of Adenine Derivatives to That of Pyrimidine Derivatives in Nearâ€0â€…eV Electronâ€Induced DNA Lesions. ChemPhysChem, 2016, 17, 1669-1677.	2.1	1
68	DNA bases ring-expanded with a cyclopentadiene free radical: a theoretical investigation of building blocks with diradical character. Organic and Biomolecular Chemistry, 2016, 14, 542-555.	2.8	7
69	Intensified effects of multi-Cu modification on the electronic properties of the modified base pairs containing hetero-ring-expanded pyrimidine bases. Physical Chemistry Chemical Physics, 2016, 18, 2913-2923.	2.8	8
70	Hydrated Electron Transfer to Nucleobases in Aqueous Solutions Revealed by Ab Initio Molecular Dynamics Simulations. ChemPhysChem, 2015, 16, 2348-2356.	2.1	9
71	Redox-Modulated Magnetic Transformations between Ferro- and Antiferromagnetism in Organic Systems: Rational Design of Magnetic Organic Molecular Switches. Journal of Physical Chemistry C, 2015, 119, 27930-27937.	3.1	26
72	Construction of reduced graphene oxide-supported Agâ€“Cu₂O composites with hierarchical structures for enhanced photocatalytic activities and recyclability. Journal of Materials Chemistry A, 2015, 3, 5923-5933.	10.3	89

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73	Computational Insights into the Charge Relaying Properties of Î²â€Turn Peptides in Protein Charge Transfers. ChemPhysChem, 2015, 16, 436-446.	2.1	4
74	Intriguing radicalâ€“radical interactions among double-electron oxidized adenineâ€“thymine base pairs. Chemical Physics Letters, 2015, 619, 223-229.	2.6	6
75	Structural fluctuation governed dynamic diradical character in pentacene. Physical Chemistry Chemical Physics, 2015, 17, 13904-13914.	2.8	8
76	Excess electron interaction with radiosensitive 5-bromopyrimidine in aqueous solution: a combined ab initio molecular dynamics and time-dependent wave-packet study. Physical Chemistry Chemical Physics, 2015, 17, 19797-19805.	2.8	8
77	Excess electron reactivity in amino acid aqueous solution revealed by ab initio molecular dynamics simulation: anion-centered localization and anion-relayed electron transfer dissociation. Physical Chemistry Chemical Physics, 2015, 17, 26854-26863.	2.8	9
78	Efficient and Substantial DNA Lesions From Near 0 eV Electron-Induced Decay of the O₄-Hydrogenated Thymine Nucleotides: A DFT Study. Journal of Physical Chemistry B, 2015, 119, 13971-13979.	2.6	2
79	Rational design of outerâ€expanded purine analogues as building blocks of DNAâ€based nanowires with enhanced electronic properties. International Journal of Quantum Chemistry, 2014, 114, 911-919.	2.0	0
80	Ab initio molecular dynamics simulations reveal localization and time evolution dynamics of an excess electron in heterogeneous CO2â€“H2O systems. Journal of Chemical Physics, 2014, 140, 044318.	3.0	15
81	Computational design of the magnetism-tunable oligobenzylic carbanion complexes. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	6
82	Glucose-Promoted Localization Dynamics of Excess Electrons in Aqueous Glucose Solution Revealed by Ab Initio Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2014, 10, 4189-4197.	5.3	9
83	Single- versus Multi-Proton-Coupled Rydberg-State Electron Transfer in Amine Clusters. Journal of Physical Chemistry C, 2014, 118, 18861-18867.	3.1	12
84	Bending Vibration-Governed Solvation Dynamics of an Excess Electron in Liquid Acetonitrile Revealed by Ab Initio Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2013, 9, 4727-4734.	5.3	11
85	Excess electron capture by hydrated histidine side-chain group. Computational and Theoretical Chemistry, 2013, 1016, 54-61.	2.5	0
86	3₁₀-Helical Peptide Acting as a Dual Relay for Charge-Hopping Transfer in Proteins. Journal of Physical Chemistry B, 2013, 117, 6385-6393.	2.6	9
87	Theoretical exploration of structures and electronic properties of double-electron oxidized guanineâ€“cytosine base pairs with intriguing radicalâ€“radical interactions. Physical Chemistry Chemical Physics, 2013, 15, 18453.	2.8	5
88	Radicalâ€“Radical Interactions among Oxidized Guanine Bases Including Guanine Radical Cation and Dehydrogenated Guanine Radicals. Journal of Physical Chemistry B, 2013, 117, 10698-10710.	2.6	6
89	Excess Dielectron in an Ionic Liquid as a Dynamic Bipolaron. Physical Review Letters, 2013, 110, 107602.	7.8	20
90	Interactions of Amino Acids with Oxidized Guanine in the Gas Phase Associated with the Protection of Damaged DNA. ChemPhysChem, 2013, 14, 1031-1042.	2.1	2

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91	Solvation and Evolution Dynamics of an Excess Electron in Supercritical<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 108, 207601.	7.8	18
92	Magnetismâ€Tunable Oligoacene Dioxide Diradicals: Promising Magnetic Oligoaceneâ€Like Molecules. ChemPhysChem, 2012, 13, 4148-4154.	2.1	4
93	A peptide loop and an Î±-helix N-terminal serving as alternative electron hopping relays in proteins. Physical Chemistry Chemical Physics, 2012, 14, 15849.	2.8	7
94	Radicalized DNA Bases through Ring-Expansion Modification: An Intriguing Class of Building Blocks for the Magnetic DNA Nanowires. Journal of Physical Chemistry C, 2012, 116, 23214-23223.	3.1	9
95	Multi-Zinc-Expanded Oligoacenes: An Intriguing Class of Well-Defined Open-Shell Singlet Diradicals. Journal of Physical Chemistry C, 2012, 116, 5900-5907.	3.1	15
96	DFT studies on the mechanism of the conversion of thiols into disulfides and dihydrogen catalyzed by CpMn(CO)3 complex. Journal of Organometallic Chemistry, 2012, 706-707, 89-98.	1.8	15
97	Multiâ€zincâ€expanded graphene patches: Tetraradical versus diradical character. Journal of Computational Chemistry, 2012, 33, 1773-1780.	3.3	9
98	Rational Design for Building Blocks of DNAâ€Based Conductive Nanowires through Multiâ€Copper Incorporation into Mismatched Base Pairs. ChemPhysChem, 2012, 13, 3293-3302.	2.1	4
99	Interaction and protection mechanism between li@C₆₀ and nucleic acid bases (NABs): Performance of PM6â€DH2 on noncovalent interaction of NABsâ€Li@C60. Journal of Computational Chemistry, 2012, 33, 490-501.	3.3	9
100	Computational design of ring-expanded pyrimidine-based DNA motifs with improved conductivity. Physical Chemistry Chemical Physics, 2011, 13, 5906.	2.8	18
101	Electronic Enhancement Effect of Copper Modification of Base Pairs on the Conductivity of DNA. Journal of Physical Chemistry C, 2011, 115, 22547-22556.	3.1	27
102	Theoretical studies on the coupling interactions in H2SO4â‹¯HOOË™â‹¯(H2O)n (n = 0â€“2) clusters: toward understanding the role of water molecules in the uptake of HOOË™ radical by sulfuric acid aerosols. Physical Chemistry Chemical Physics, 2011, 13, 941-953.	2.8	10
103	Multi-Copper-Mediated DNA Base Pairs Acting as Suitable Building Blocks for the DNA-Based Nanowires. Journal of Physical Chemistry C, 2011, 115, 2855-2864.	3.1	16
104	Electronic promotion effect of double proton transfer on conduction of DNA through improvement of transverse electronic communication of base pairs. Journal of Chemical Physics, 2011, 135, 134315.	3.0	15
105	On the Binding Strength Sequence for Nucleic Acid Bases and C60 with Density Functional and Dispersion-Corrected Density Functional Theories: Whether C60 Could Protect Nucleic Acid Bases from Radiation-Induced Damage. Journal of Physical Chemistry C, 2011, 115, 3220-3228.	3.1	26
106	Internucleotide Jâ€couplings and chemical shifts of the Nï£¿HÂ·Â·Â·N hydrogenâ€bonds in the radiationâ€damaged guanineâ€cytosine base pairs. Journal of Computational Chemistry, 2011, 32, 1159-1169.	3.3	6
107	Absorption and fluorescence emission spectroscopic characters of naphthoâ€homologated yyâ€DNA bases and effect of methanol solution and base pairing. Journal of Computational Chemistry, 2010, 31, 825-836.	3.3	14
108	Peptides-assisted charge transfers in proteins: relay mechanism and its controllability. Frontiers of Chemistry in China: Selected Publications From Chinese Universities, 2010, 5, 309-324.	0.4	0

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109	Coupling Interactions between Sulfurous Acid and the Hydroperoxyl Radical. ChemPhysChem, 2010, 11, 696-705.	2.1	9
110	Redoxâ€induced configuration conversion for thioacetamide dimer can function as a molecular switch. Journal of Computational Chemistry, 2010, 31, 2533-2539.	3.3	4
111	Tethered-Hopping Model for Protein-DNA Binding and Unbinding Based on Sox2-Oct1-Hoxb1 Ternary Complex Simulations. Biophysical Journal, 2010, 98, 1285-1293.	0.5	16
112	Negative Dissociation Energy Phenomenon of Metastable H-Bonds As Revealed in Triplex DNA Hole Migration. Journal of Physical Chemistry B, 2010, 114, 1144-1147.	2.6	7
113	Î±-Helix C-Terminus Acting as a Relay to Mediate Long-Range Hole Migration in Proteins. Journal of Physical Chemistry Letters, 2010, 1, 1637-1641.	4.6	33
114	The capture of Ë™H and Ë™OH radicals by vitamin C and implications for the new source for the formation of the anion free radical. Physical Chemistry Chemical Physics, 2010, 12, 5256.	2.8	18
115	States and migration of an excess electron in a pyridinium-based, room-temperature ionic liquid: an ab initio molecular dynamics simulation exploration. Physical Chemistry Chemical Physics, 2010, 12, 1854.	2.8	28
116	Unexpected dissociation energetics of the Na+ counterion from GC motifs in DNA hole-migration. Physical Chemistry Chemical Physics, 2010, 12, 13099.	2.8	3
117	Molecular dynamics simulation exploration of cooperative migration mechanism of calcium ions in sarcoplasmic reticulum Ca²⁺â€ATPase. Journal of Computational Chemistry, 2009, 30, 2136-2145.	3.3	13
118	Effect of metal ions on radical type and protonâ€coupled electron transfer channel: Ïƒâ€Radical vs Ïâ€radical and Ïƒâ€channel vs Ïâ€channel in the imide units. Journal of Computational Chemistry, 2009, 30, 2694-2705.	3.3	12
119	Theoretical studies of the proton transfer behaviors in molecular complexes analogous to catalytic triad of serine protease: Toward understanding the existence and significance of the low-barrier hydrogen-bond in enzymatic catalysis. Science in China Series B: Chemistry, 2009, 52, 131-136.	0.8	2
120	Theoretical prediction of sizeâ€expansion effect on the C8â€site activity in the modified guanineâ€cytosine analogs. Journal of Physical Organic Chemistry, 2009, 22, 1114-1119.	1.9	6
121	Excess Electron Solvation in an Imidazolium-Based Room-Temperature Ionic Liquid Revealed by Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 8222-8226.	2.6	42
122	Proton-Regulated Electron Transfers from Tyrosine to Tryptophan in Proteins: Through-Bond Mechanism versus Long-Range Hopping Mechanism. Journal of Physical Chemistry B, 2009, 113, 16681-16688.	2.6	23
123	Hetero-Ring-Expansion Design for Adenine-Based DNA Motifs: Evidence from DFT Calculations and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 4407-4412.	2.6	29
124	Probing the imine silylenoid HN=SiNaF and its insertions reaction with Râ€“H (R=F, OH, NH2, CH3) using DFT. Structural Chemistry, 2008, 19, 527-533.	2.0	6
125	Theoretical studies on the properties of uracil and its dimer upon thioketo substitution. Theoretical Chemistry Accounts, 2008, 121, 21-31.	1.4	4
126	Isomerization of HNO to HON in the singlet state assisted by amino acid residues and/or water molecules. International Journal of Quantum Chemistry, 2008, 108, 1246-1256.	2.0	1

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127	Photophysical Characters of Rationally Designed Hetero-Ring-Expanded Guanine Analogues and Effect of Cytosine Pairing. Journal of Physical Chemistry B, 2008, 112, 10723-10731.	2.6	20
128	Remarkable Metal Counterion Effect on the Internucleotide J-Couplings and Chemical Shifts of the Nâ^'HÂ·Â·Â·N Hydrogen Bonds in the Wâ^'C Base Pairs. Journal of Physical Chemistry B, 2008, 112, 9174-9181.	2.6	10
129	Solvation of Excess Electrons in LiF Ionic Pair Matrix:â€‰ Evidence for a Solvated Dielectron from Ab Initio Molecular Dynamics Simulations and Calculations. Journal of Physical Chemistry B, 2008, 112, 3767-3772.	2.6	18
130	Relay Stations for Electron Hole Migration in Peptides: Possibility for Formation of Three-Electron Bonds along Peptide Chains. Journal of Physical Chemistry B, 2008, 112, 14302-14311.	2.6	28
131	Rational Design of Hetero-ring-Expanded Guanine Analogs with Enhanced Properties for Modified DNA Building Blocks. Journal of Physical Chemistry B, 2007, 111, 8335-8341.	2.6	35
132	Pairing strength and proton characters of the N7,N9-dimethylated GC and AT base pairs: a density functional theory investigation. New Journal of Chemistry, 2007, 31, 1514.	2.8	4
133	Cation-Modulated Electron-Transfer Channel:Â H-Atom Transfer vs Proton-Coupled Electron Transfer with a Variable Electron-Transfer Channel in Acylamide Units. Journal of the American Chemical Society, 2007, 129, 9713-9720.	13.7	29
134	Exploration of the Ca2+ Interaction Modes of the Nifedipine Calcium Channel Antagonist. ChemPhysChem, 2007, 8, 304-314.	2.1	4
135	Exploration on Regulating Factors for Proton Transfer along Hydrogen-Bonded Water Chains. ChemPhysChem, 2007, 8, 944-954.	2.1	17
136	Selective Synthesis and Luminescent Properties of Monazite- and Zircon-Type LaVO₄:Ln (Ln) Tj ETQq0 0 0 rgBT /Overlock 1	3.0	72
137	Hydration effect on interaction mode between glutamic acid and Ca2+ and its biochemical implication: a theoretical exploration. New Journal of Chemistry, 2006, 30, 890.	2.8	2
138	Proton Character of the Peptide Unit in the Ca2+-Binding Sites of Calcium Pump. Journal of Physical Chemistry B, 2006, 110, 11005-11013.	2.6	11
139	Different catalysis role of in-loop and out-of-loop waters in assisting HNS/HSN proton transfer isomerizations: Bridging vs. surrounding effect. International Journal of Quantum Chemistry, 2006, 106, 1528-1543.	2.0	2
140	Properties and isomerization mechanism of the singlet state imidazoleâ€“imidazolium system. Computational and Theoretical Chemistry, 2006, 758, 1-8.	1.5	1
141	Coupling characteristics and proton transfer mechanisms of guanineâ€“Na+ monohydrate. Computational and Theoretical Chemistry, 2006, 760, 209-217.	1.5	7
142	Electron bridging dihydrogen bond in the imidazole-contained anion derivatives. Journal of Chemical Physics, 2006, 124, 124314.	3.0	11
143	The regulatory roles of metal ions (M+/2+= Li+, Na+, K+, Be2+, Mg2+, and Ca2+) and water molecules in stabilizing the zwitterionic form of glycine derivatives. New Journal of Chemistry, 2005, 29, 1540.	2.8	19
144	Double proton transfer and one-electron oxidation behavior in double H-bonded glycinamide-glycine complex in the gas phase. Journal of Computational Chemistry, 2005, 26, 552-560.	3.3	1

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145	Theoretical prediction of the contact distance dependence of the electron transfer reactivity of the ClO/ClO? coupling system. International Journal of Quantum Chemistry, 2005, 101, 305-319.	2.0	1
146	Hydrogen bond character and proton transfer behavior in water-thiophenol clusters and their cation radicals: Insight into water number size dependence. International Journal of Quantum Chemistry, 2005, 105, 186-198.	2.0	2
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