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	Dual-atom Pt heterogeneous catalyst with excellent catalytic performances for the selective hydrogenation and epoxidation. Nature Communications, 2021, 12, 3181.	12.8	156
2	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
3	Selective Synthesis and Luminescent Properties of Monazite- and Zircon-Type LaVO₄:Ln (Ln) Tj ETQq1 1 0.784314 rgBT	3.0	72
4	Glycine-Zn+/Zn2+ and their hydrates: On the number of water molecules necessary to stabilize the switterionic glycine-Zn+/Zn2+ over the nonzwitterionic ones. Journal of Chemical Physics, 2003, 118, 10973-10985.	3.0	48
5	Theoretical Determinations of Ionization Potential and Electron Affinity of Glycinamide Using Density Functional Theory. Journal of Physical Chemistry A, 2004, 108, 1200-1207.	2.5	44
6	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
7	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
8	Coupling Character between Imidazole and Imidazole Cation:Â Implication for the Coupling Modes of Biomolecular Residues. Journal of Physical Chemistry A, 2004, 108, 7038-7049.	2.5	36
9	Facile and economical synthesis of ZnS nanotubes and their superior adsorption performance for organic dyes. CrystEngComm, 2017, 19, 2380-2393.	2.6	36
10	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
11	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
12	Conformational Study of Glycine Amide Using Density Functional Theory. Journal of Physical Chemistry A, 2003, 107, 6419-6428.	2.5	30
13	Theoretical Study of Landauâ€“Zener Electronic Transmission Factor for Outer-Sphere Electron Transfer Reactions in Solution. The Journal of Physical Chemistry, 1996, 100, 18093-18100.	2.9	29
14	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
15	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
16	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
17	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
18	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

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19	Regio- and Diastereoselective Cross-Dehydrogenative Coupling of Tetrahydropyridines with 1,3-Dicarbonyl Compounds. Organic Letters, 2017, 19, 2146-2149.	4.6	27
20	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
21	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
22	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
23	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
24	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
25	Hydration Model for the Energy Barrier in Self-Exchange Electron Transfer Reactions in Solution. Journal of Physical Chemistry A, 1997, 101, 1198-1205.	2.5	22
26	Marked Variations of Dissociation Energy and H-Bond Character of the Guanine-Cytosine Base Pair Induced by One-Electron Oxidation and Li+Cation Coupling. Journal of Physical Chemistry B, 2005, 109, 593-600.	2.6	22
27	Structure and property of glycineâ€™s derivatives bound by multications (H+, Li+, and Na+): A theoretical study. Journal of Chemical Physics, 2002, 117, 7593-7602.	3.0	21
28	Alteration of Imidazole Dimer on Oxidation or Water Ligation. Journal of Physical Chemistry B, 2004, 108, 13874-13881.	2.6	21
29	Theoretical investigation of glycineâ€“2Ben+ (n=0,1,2) complexes in gas phase: Origin of negative dissociation energies. Journal of Chemical Physics, 2003, 118, 1761-1772.	3.0	20
30	Density Functional Studies on Conformational Behaviors of Glycinamide in Solution. Journal of Physical Chemistry B, 2004, 108, 1405-1413.	2.6	20
31	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
32	Excess Dielectron in an Ionic Liquid as a Dynamic Bipolaron. Physical Review Letters, 2013, 110, 107602.	7.8	20
33	Reduced graphene oxide-stabilized copper nanocrystals with enhanced catalytic activity and SERS properties. RSC Advances, 2016, 6, 50587-50594.	3.6	20
34	Polymeric tungsten carbide nanoclusters: structural evolution, ligand modulation, and assembled nanomaterials. Nanoscale, 2019, 11, 19903-19911.	5.6	20
35	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
36	Multiwater-Assisted Proton Transfer Study in Glycinamide Using Density Functional Theory. Journal of Physical Chemistry B, 2004, 108, 18088-18097.	2.6	18

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37	Geometry and binding properties of different multiple-state glycine-Fe+/Fe2+ complexes. Journal of Physical Organic Chemistry, 2005, 18, 26-34.	1.9	18
38	Structural Character and Energetics of Tyrosyl Radical Formation by Electron/Proton Transfers of a Covalently Linked Histidine-Tyrosine:Â A Model for CytochromecOxidase. Journal of Physical Chemistry B, 2005, 109, 22013-22026.	2.6	18
39	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
40	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
41	Computational design of ring-expanded pyrimidine-based DNA motifs with improved conductivity. Physical Chemistry Chemical Physics, 2011, 13, 5906.	2.8	18
42	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
43	Dynamics Insight into Isomerization and Dissociation of Hot Criegee Intermediate CH3CHOO. Journal of Physical Chemistry A, 2019, 123, 1085-1090.	2.5	18
44	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
45	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
46	Exploration on Regulating Factors for Proton Transfer along Hydrogen-Bonded Water Chains. ChemPhysChem, 2007, 8, 944-954.	2.1	17
47	Protonation-Enhanced Antiferromagnetic Couplings in Azobenzene-Bridged Diradicals. Journal of Physical Chemistry C, 2017, 121, 17160-17168.	3.1	17
48	Intramolecular proton transfer induced by divalent alkali earth metal cation in the gas state. International Journal of Quantum Chemistry, 2003, 94, 205-214.	2.0	16
49	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
50	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
51	Core-Modified Porphyrin Diradicals with a Cî•€ Unit: Redox-Driven Magnetic Switching. Journal of Physical Chemistry C, 2017, 121, 21231-21243.	3.1	16
52	Hydrates of the most stable gas-phase mono- and di-protonated glycine derivatives: Origin of no reservation energy bond in glycine-2H2+. Journal of Chemical Physics, 2004, 120, 2208-2214.	3.0	15
53	Acidâ^'Base Behavior Study of Glycinamide Using Density Functional Theory. Journal of Physical Chemistry A, 2004, 108, 4069-4079.	2.5	15
54	Investigations of Double Proton Transfer Behavior between Glycinamide and Formamide Using Density Functional Theory. Journal of Physical Chemistry A, 2004, 108, 10288-10295.	2.5	15

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55	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
56	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
57	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
58	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
59	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
60	The Coupling Character of Ca2+ with Glutamic Acid:â€‰ Implication for the Conformational Behavior and Transformation of Ca2+-ATPase in Transmembrane Ca2+ Channel. Journal of Physical Chemistry B, 2004, 108, 17628-17638.	2.6	14
61	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
62	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
63	Theoretical prediction of the structures and properties of cyclic AlS2 and GaS2 systems at density functional theory and all-electron correlation levels. Chemical Physics Letters, 2000, 319, 725-732.	2.6	13
64	The bonding character of the cyclic AlSO and GaSO species: ab initio investigations at density functional theory and the electron correlation levels. Chemical Physics Letters, 2000, 322, 503-512.	2.6	13
65	Theoretical prediction of the stateâ€“state correlation among doublet state AlSO isomers. Chemical Physics Letters, 2001, 338, 142-150.	2.6	13
66	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
67	Ab initio studies on hydrogen-transfer tunneling for Cl + HCl abstraction hydrogen reaction. International Journal of Quantum Chemistry, 1996, 57, 95-104.	2.0	12
68	Coupling properties of imidazole dimer radical cation assisted by embedded water molecule: Toward understanding of interaction character of hydrogen-bonded histidine residue side-chains. Journal of Chemical Physics, 2005, 122, 184324.	3.0	12
69	Effect of metal ions on radical type and protonâ€coupled electron transfer channel: Ïƒâ€Radical vs Ï€â€radical and Ïƒâ€channel vs Ï€â€channel in the imide units. Journal of Computational Chemistry, 2009, 30, 2694-2705.	3.3	12
70	Single- versus Multi-Proton-Coupled Rydberg-State Electron Transfer in Amine Clusters. Journal of Physical Chemistry C, 2014, 118, 18861-18867.	3.1	12
71	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
72	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

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73	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
74	Bonding and Correlation Analysis of Various SiCO Isomers. Journal of Physical Chemistry A, 2002, 106, 11897-11910.	2.5	11
75	Theoretical Studies for the Structural Properties and Electron Transfer Reactivity of C4H5N/C4H5N+Coupling System. Journal of Physical Chemistry A, 2003, 107, 1584-1596.	2.5	11
76	Reservation Energy Bonds and Structural Stability of Series of Multihydrated (nH2O = 1â^'10) Glycineâ^'H+M+ (M = Li, Na, or K) Complexes. Journal of Physical Chemistry B, 2004, 108, 1241-1254.	2.6	11
77	Effects of Donors and Acceptors on the Energetics and Mechanism of Proton, Hydrogen, and Hydride Release from Imidazole. Journal of Physical Chemistry B, 2004, 108, 10089-10100.	2.6	11
78	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
79	Electron bridging dihydrogen bond in the imidazole-contained anion derivatives. Journal of Chemical Physics, 2006, 124, 124314.	3.0	11
80	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
81	Molecular Vibrations Induced Potential Diradical Character in Hexazapentacene. Journal of Physical Chemistry C, 2016, 120, 10215-10226.	3.1	11
82	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
83	Organic ligand mediated evolution from aluminum-based superalkalis to superatomic molecules and one-dimensional nanowires. Nano Research, 2022, 15, 1162-1170.	10.4	11
84	Nonempirical ab initio studies on inner-sphere reorganization energies of M2+(H2O)6/M3+(H2O)6 redox couples at valence basis level. International Journal of Quantum Chemistry, 1997, 61, 117-126.	2.0	10
85	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
86	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
87	Unusual Indirect Nuclear Spinâ€“Spin Exchange Coupling through Solvated Electron. Journal of Physical Chemistry Letters, 2018, 9, 689-695.	4.6	10
88	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
89	Theoretical Study of V2+OH2/V3+OH2Electron Transfer Reactivity at Electron Correlation Level. Journal of Physical Chemistry A, 1999, 103, 4485-4493.	2.5	9
90	Structural analysis of the cyclic AlO2 and AlS2 systems in doublet and quartet states at density functional theory and the electron correlation levels. Journal of Chemical Physics, 2000, 113, 4216-4229.	3.0	9

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91	Theoretical prediction of the stateâ€“state correlation among doublet state SNO isomers. Chemical Physics Letters, 2003, 370, 616-624.	2.6	9
92	Coupling Interactions between Sulfurous Acid and the Hydroperoxyl Radical. ChemPhysChem, 2010, 11, 696-705.	2.1	9
93	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
94	Multiâ€zincâ€expanded graphene patches: Tetraradical versus diradical character. Journal of Computational Chemistry, 2012, 33, 1773-1780.	3.3	9
95	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
96	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
97	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
98	Hydrated Electron Transfer to Nucleobases in Aqueous Solutions Revealed by Ab Initio Molecular Dynamics Simulations. ChemPhysChem, 2015, 16, 2348-2356.	2.1	9
99	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
100	Tuning the Spin Coupling Interactions in the Nitroxideâ€Based Bisphenolâ€Like Diradicals. ChemPhysChem, 2017, 18, 2487-2498.	2.1	9
101	Marked Increments of Stability and Proton Affinity of the Protonated, Zwitterionic Glycine Induced by the Attachment of Two Excess Electrons. Journal of Physical Chemistry A, 2004, 108, 4156-4162.	2.5	8
102	Electronic effect on protonated hydrogen-bonded imidazole trimer and corresponding derivatives cationized by alkali metals (Li+, Na+, and K+). Journal of Chemical Physics, 2005, 122, 054311.	3.0	8
103	Structural fluctuation governed dynamic diradical character in pentacene. Physical Chemistry Chemical Physics, 2015, 17, 13904-13914.	2.8	8
104	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
105	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
106	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
107	Golden-rule treatment of the O2+Oâ^'2 electron-transfer reaction. Computational and Theoretical Chemistry, 1999, 459, 177-186.	1.5	7
108	Theoretical approaches of the isomerization mechanism of GaSO isomers in doublet states at density functional theory levels. Chemical Physics, 2001, 273, 103-115.	1.9	7

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109	Theoretical study of the structural character of weakly bonding silicon carbonyl complexes. Theoretical Chemistry Accounts, 2002, 108, 293-304.	1.4	7
110	Theoretical study of the pyridineâ€“BF3 complex. Computational and Theoretical Chemistry, 2002, 588, 1-8.	1.5	7
111	Coupling characteristics and proton transfer mechanisms of guanineâ€“Na+ monohydrate. Computational and Theoretical Chemistry, 2006, 760, 209-217.	1.5	7
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	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
114	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
115	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
116	Proton-Transfer-Regulated Magnetic Spin Couplings in Nitroxide-Functionalized Porphycene Diradicaloids. Journal of Physical Chemistry C, 2019, 123, 10764-10776.	3.1	7
117	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
118	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
119	Theoretical investigation of the cyclic GaO2 and GaS2 molecules at DFT and correlated wave function levels. International Journal of Quantum Chemistry, 2001, 81, 222-231.	2.0	6
120	Double proton transfer behavior and one-electron oxidation effect in double H-bonded glycinamide-formic acid complex. Journal of Chemical Physics, 2004, 121, 9971-9981.	3.0	6
121	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
122	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
123	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
124	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
125	Computational design of the magnetism-tunable oligobenzylic carbanion complexes. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	6
126	Intriguing radicalâ€“radical interactions among double-electron oxidized adenineâ€“thymine base pairs. Chemical Physics Letters, 2015, 619, 223-229.	2.6	6

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127	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
128	Ab initio time-dependent perturbation study of tunnelling effect in the abstraction of hydrogen from methane by methyl radical. Computational and Theoretical Chemistry, 1997, 417, 69-80.	1.5	5
129	Structure and property study of the O2 + O2â˙ electron transfer system. Computational and Theoretical Chemistry, 1998, 429, 143-151.	1.5	5
130	The structural character of AlS2 species in quartet state: prediction at density functional theory and the correlated-wave function levels. Chemical Physics, 2001, 271, 229-238.	1.9	5
131	Double Proton Transfer and One-Electron Oxidation Behaviors in Double H-Bonded Glycinamideâ˙Formamidine Complex and Comparison with Biological Base Pair. Journal of Physical Chemistry B, 2004, 108, 16976-16982.	2.6	5
132	Timeâ€dependent treatment of intramolecular energy transfer for HeICl complex. Chinese Journal of Chemistry, 1997, 15, 218-224.	4.9	5
133	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
134	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
135	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
136	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
137	Cr2+OH2/Cr3+OH2 electron transfer reactivity: an ab initio study at UMP2/6-311+G* level including all electron correlation. Computational and Theoretical Chemistry, 1999, 489, 141-149.	1.5	4
138	The bonding character of AlSO isomers in quartet excited states: Ab initio and density functional theory studies. International Journal of Quantum Chemistry, 2002, 87, 181-191.	2.0	4
139	Water-Assisting Proton Transfer Isomerization of the HNO/HON System in the Singlet State:â€‰ On the Number of the Effective Water Molecules. Journal of Physical Chemistry B, 2004, 108, 11732-11743.	2.6	4
140	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
141	Exploration of the Ca2+ Interaction Modes of the Nifedipine Calcium Channel Antagonist. ChemPhysChem, 2007, 8, 304-314.	2.1	4
142	Theoretical studies on the properties of uracil and its dimer upon thioketo substitution. Theoretical Chemistry Accounts, 2008, 121, 21-31.	1.4	4
143	Redoxâ€induced configuration conversion for thioacetamide dimer can function as a molecular switch. Journal of Computational Chemistry, 2010, 31, 2533-2539.	3.3	4
144	Magnetismâ€Tunable Oligoacene Dioxide Diradicals: Promising Magnetic Oligoaceneâ€Like Molecules. ChemPhysChem, 2012, 13, 4148-4154.	2.1	4

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145	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
146	Computational Insights into the Charge Relaying Properties of Î²â€Turn Peptides in Protein Charge Transfers. ChemPhysChem, 2015, 16, 436-446.	2.1	4
147	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
148	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
149	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
150	Dielectron Clathrate Hydrates with Unique Superexchange Spin Couplings. Journal of Physical Chemistry C, 2018, 122, 7635-7641.	3.1	4
151	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
152	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
153	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
154	Intriguing electric field effect on magnetic spin couplings in dielectron clathrate hydrates. International Journal of Quantum Chemistry, 2019, 119, e25916.	2.0	4
155	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
156	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
157	Dual External Field-Engineered Hyperhalogen. Journal of Physical Chemistry Letters, 2022, 13, 3942-3948.	4.6	4
158	Theoretical studies on the inner-sphere reorganization energies for the self-exchange reactions of gas-phase diatomic molecules HA (A = Mg, Al, Si, P, S, Cl). International Journal of Quantum Chemistry, 1995, 54, 249-259.	2.0	3
159	Electron transfer reactivity of O2+O2? system in low-spin coupling:Ab Initio study at electron correlation level. Journal of Computational Chemistry, 1999, 20, 989-998.	3.3	3
160	Ab initio prediction of Mn2+OH2/Mn3+OH2 electron transfer reactivity at electron correlation level. Computational and Theoretical Chemistry, 2000, 530, 327-341.	1.5	3
161	Theoretical study on the ClO/ClOâ¯ system electron-transfer reactivity by the Golden-rule. Computational and Theoretical Chemistry, 2003, 629, 105-115.	1.5	3
162	Structures and positive binding energies of glycineâ€“2Li+ in the gas phase: a theoretical study on optimal reaction pathway and proton transfer induced by two lithium cations. Computational and Theoretical Chemistry, 2004, 678, 91-103.	1.5	3

#	Article	IF	Citations
163	Unexpected dissociation energetics of the Na+ counterion from GC motifs in DNA hole-migration. Physical Chemistry Chemical Physics, 2010, 12, 13099.	2.8	3
164	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
165	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
166	Cu-wire-mediatedÂdipyrimidineÂbaseÂpairsÂasÂthe buildingÂblocksÂforÂ conductive and magnetic Cuâ€“DNAÂ nanowires. Journal of Mathematical Chemistry, 2017, 55, 1301-1321.	1.5	3
167	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
168	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
169	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
170	Dynamic relaying properties of a Î²â€turn peptide in longâ€range electron transfer. Journal of Computational Chemistry, 2019, 40, 988-996.	3.3	3
171	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
172	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
173	Golden-rule treatment on the ClO/ClO+ electron-transfer system. Computational and Theoretical Chemistry, 2003, 629, 151-163.	1.5	2
174	Theoretical studies on structural properties and electron transfer reactivity of the C4H4O/C4H4O+ furan coupling pair. Computational and Theoretical Chemistry, 2004, 671, 161-172.	1.5	2
175	Structures and bonding character of cyclic AsO2 and AsS2 systems in the doublet state. Chemical Physics Letters, 2004, 387, 160-164.	2.6	2
176	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
177	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
178	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
179	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
180	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

#	Article	IF	Citations
181	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
182	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
183	Nonlinear Migration Dynamics of Excess Electrons along Linear Oligopeptides Controlled by an Applied Electric Field. ChemPhysChem, 2019, 20, 1497-1507.	2.1	2
184	Electric field controlled uphill electron migration along Î±-helical oligopeptides. Physical Chemistry Chemical Physics, 2021, 23, 1464-1474.	2.8	2
185	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
186	Intriguing strain-governed magnetic phase transitions in 2D vanadium porphyrin sheets. Physical Chemistry Chemical Physics, 2022, 24, 3834-3843.	2.8	2
187	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
188	The inner-sphere reorganization energies for AH2 + AH2+(?) (A = Al, Si, P, S) electron self-exchange reactions in electron-transfer processes from ab initio calculations. International Journal of Quantum Chemistry, 1995, 55, 329-337.	2.0	1
189	Theoretical study of the inner-sphere energy barrier of the transition-metal complex M(H2O)62+/3+ in electron-transfer process. International Journal of Quantum Chemistry, 1999, 75, 119-126.	2.0	1
190	The orientation and distance-dependence analysis of the electron transfer reactivity: An electron correlation level investigation of Mn2+(H2O)2/Mn3+(H2O)2 system. Journal of Computational Chemistry, 2000, 21, 1387-1404.	3.3	1
191	Theoretical studies on the contact distance dependence of the electron transfer reactivity of the ClO/ClO+ coupling system. New Journal of Chemistry, 2003, 27, 1012.	2.8	1
192	Structure analysis of [P,N,O] species in singlet and triplet states at density functional theory and wavefunction-correlated levels. Computational and Theoretical Chemistry, 2004, 668, 163-169.	1.5	1
193	Structures and properties of [CNâ‹¯CNâ‹¯] coupling system in doublet state. Computational and Theoretical Chemistry, 2004, 677, 39-49.	1.5	1
194	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
195	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
196	Properties and isomerization mechanism of the singlet state imidazoleâ€“imidazolium system. Computational and Theoretical Chemistry, 2006, 758, 1-8.	1.5	1
197	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
198	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

#	Article	IF	Citations
199	Unique Solvating Effect in Azabenzene Clathrate Hydrates. Journal of Physical Chemistry C, 2018, 122, 28466-28477.	3.1	1
200	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
201	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
202	Theoretical investigation of the cyclic GaO2 and GaS2 molecules at DFT and correlated wave function levels. International Journal of Quantum Chemistry, 2001, 81, 222-231.	2.0	1
203	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
204	Effect of different subsets on convergence patterns of hyperspherical harmonic expansion for theS states of the helium atom. International Journal of Quantum Chemistry, 1997, 64, 661-668.	2.0	0
205	Theoretical sstudy on the Co2+OH2+/Co3+OH2+ electron transfer reactivity. Science in China Series B: Chemistry, 2001, 44, 234-245.	0.8	0
206	Structure analysis of SiSO+ and GeSO+ systems in doublet state at density functional theory and wavefunction-correlated levels. Chemical Physics Letters, 2003, 377, 462-468.	2.6	0
207	Electron transfer reactivity of methyl-substituted amine NHn(CH3)3?n/NHn(CH3)3?n+ (n = 0-3) self-exchange systems: a theoretical investigation. Journal of Physical Organic Chemistry, 2005, 18, 69-82.	1.9	0
208	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
209	Electronic factor in electron selfâ€exchange reaction of hydrated redox ion pairs from thermodynamic data. Chinese Journal of Chemistry, 1997, 15, 201-210.	4.9	0
210	Novel Bonding Character of the Cyclic AlS₂ and GaS₂ Systems. Chinese Journal of Chemistry, 2001, 19, 637-640.	4.9	0
211	Excess electron capture by hydrated histidine side-chain group. Computational and Theoretical Chemistry, 2013, 1016, 54-61.	2.5	0
212	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
213	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
214	Hydroxide-Enhanced Superexchange Magnetic Couplings in Ionic Clathrate Hydrates. Journal of Physical Chemistry C, 2020, 124, 25455-25464.	3.1	0
215	Molecular dynamics insights into electron-catalyzed dissociation repair of cyclobutane pyrimidine dimer. Chinese Journal of Chemical Physics, 2021, 34, 850-860.	1.3	0