Xu-ri Huang

List of Publications by Year
in descending order

143 papers	2,252 citations	304743 22 h-index	243625 44 g-index
143 all docs	143 docs citations	143 times ranked	3470 citing authors

#	Article	IF	Citations
1	Catalytic activity of Ruâ€N₄ doped vacancy fullerenes (Ruâ€N₄â€C₅₄) Tj ETQq1 1 0.784314 rgB theory investigation. Applied Organometallic Chemistry, 2022, 36, .	3.5	2
2	Realizing Efficient Catalytic Performance and High Selectivity for Oxygen Reduction Reaction on a 2D Ni₂SbTe₂ Monolayer. Inorganic Chemistry, 2022, 61, 2284-2291.	4.0	7
3	Heteroatom-doped fullerene C70 as non-metal electrocatalysts for oxygen reduction and oxygen evolution from computational study. Diamond and Related Materials, 2022, 124, 108954.	3.9	3
4	The Reaction Mechanism Study for the F3 System. BioMed Research International, 2022, 2022, 1-7.	1.9	0
5	Generation of singlet oxygen catalyzed by the room-temperature-stable anthraquinone anion radical. Physical Chemistry Chemical Physics, 2022, 24, 14165-14171.	2.8	2
6	Accurate Adiabatic and Diabatic Potential Energy Surfaces for the Reaction of He + H2. BioMed Research International, 2022, 2022, 1-15.	1.9	0
7	The binding process of BmKTX and BmKTX-D33H toward to Kv1.3 channel: a molecular dynamics simulation study. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2788-2797.	3.5	1
8	Theoretical Study on a Potential Oxygen Reduction Reaction Electrocatalyst: Single Fe Atoms Supported on Graphite Carbonitride. Langmuir, 2021, 37, 428-436.	3.5	9
9	Probing the activity of transition metal M and heteroatom N₄ co-doped in vacancy fullerene (Mâ€“N₄â€“C₆₄, M = Fe, Co, and Ni) towards the oxygen reduction reaction by density functional theory. RSC Advances, 2021, 11, 3174-3182.	3.6	11
10	Ironâ€Catalyzed Nâ€Alkylation of Secondary Amines with Alcohols Using Borrowing Hydrogen Strategy. ChemistrySelect, 2021, 6, 4089-4097.	1.5	1
11	Mechanistic Insight into Pd(II)-Catalyzed Late-Stage Nondirected C(sp²)â€“H Cyanation of Toluene Using the Dual Ligands MPAA and Quinoxaline: A Density Functional Theory Investigation. Journal of Organic Chemistry, 2021, 86, 10526-10535.	3.2	1
12	Metal-ionic-conductor potassium ferrite nanocrystals with intrinsic superhydrophilic surfaces for electrocatalytic water splitting at ultrahigh current densities. Journal of Materials Chemistry A, 2021, 9, 7586-7593.	10.3	40
13	Applying surface strain and coupling with pure or N/B-doped graphene to successfully achieve high HER catalytic activity in 2D layered SnP₃-based nanomaterials: a first-principles investigation. Inorganic Chemistry Frontiers, 2020, 7, 647-658.	6.0	22
14	Global accurate diabatic potential surfaces for the reaction H + Li₂. RSC Advances, 2020, 10, 39226-39240.	3.6	5
15	Activity adaptability of a DhHP-6 peroxidase-mimic in wide pH and temperature ranges and solvent media. Catalysis Science and Technology, 2020, 10, 1848-1857.	4.1	5
16	Embedding tetrahedral 3d transition metal TM₄ clusters into the cavity of two-dimensional graphdiyne to construct highly efficient and nonprecious electrocatalysts for hydrogen evolution reaction. Physical Chemistry Chemical Physics, 2020, 22, 3254-3263.	2.8	20
17	Exploring the Mechanism of the Palladium-Catalyzed 3-Butene-2-ol Amination Reaction: A DFT Study. Frontiers in Chemistry, 2020, 8, 48.	3.6	2
18	Theoretical study of a novel organic electride with large nonlinear optical responses. International Journal of Quantum Chemistry, 2020, 120, e26235.	2.0	3

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19	Computational study on C1- versus C3-regioselectivity in Pd(II)-catalyzed olefination/dearomatization of 2-naphthyl ureas. Molecular Catalysis, 2019, 477, 110540.	2.0	0
20	Theoretical investigation on the structures, electronic and magnetic properties of new 2D/1D composite nanosystems by adsorbing superhalogen MnCl3 on the BN monolayer/nanoribbons. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	3
21	Theoretical study of the photochemical isomerization process of perfluoroaryltetrahedrane to perfluoroarylcyclobutadiene mediated by 9,10-dicyanoanthracene. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	0
22	An accurate ground state potential surface for the scattering reaction F^{â˜} + F₂(v,j) â† F₂(vâ€²,jâ€²) + F^{â˜}. RSC Advances, 2019, 9, 1929-1932.	2.6	7
23	Methanol dissociation and oxidation on single Fe atom supported on graphitic carbon nitride. Applied Organometallic Chemistry, 2019, 33, e4930.	3.5	5
24	Theoretical study of substituent effects on electride characteristics and the nonlinear optical properties of Li@calix[4]pyrrole. RSC Advances, 2019, 9, 37919-37925.	3.6	5
25	Molecular dynamics simulations investigate the pathway of substrate entry active site of rhomboid protease. Journal of Biomolecular Structure and Dynamics, 2019, 37, 3445-3455.	3.5	5
26	Adsorbing the magnetic superhalogen MnCl₃ to realize intriguing half-metallic and spin-gapless-semiconducting behavior in zigzag or armchair SiC nanoribbon. RSC Advances, 2018, 8, 13167-13177.	3.6	6
27	Methanol activation catalyzed by Pt₇, Pt₃Cu₄, and Cu₇ clusters: A density functional theory investigation. Applied Organometallic Chemistry, 2018, 32, e4197.	3.5	10
28	Elucidating proton-mediated conformational changes in an acid-sensing ion channel 1a through molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2018, 36, 2261-2267.	3.5	1
29	Conformational transitions of uracil transporter UraA from Escherichia coli: a molecular simulation study. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3398-3410.	3.5	1
30	Hostâ€“Guest Interaction Creates Hydrogen-Evolution Electrocatalytic Active Sites in 3d Transition Metal-Intercalated Titanates. ACS Applied Materials & Interfaces, 2018, 10, 696-703.	8.0	17
31	Molecular dynamics simulations investigate the mechanism of Psalmotoxin 1 regulating gating process of an acid-sensing ion channel 1a at pH 5.5. Journal of Biomolecular Structure and Dynamics, 2018, 36, 2558-2566.	3.5	2
32	Efficient oxygen evolution electrocatalysis in acid by a perovskite with face-sharing IrO6 octahedral dimers. Nature Communications, 2018, 9, 5236.	12.8	325
33	Reaction of CO₂ with Atomic Transition Metal M^{+/0/â€“} Ions: A Theoretical Study. Journal of Physical Chemistry A, 2018, 122, 5848-5860.	2.5	10
34			

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37	Accurate potential energy surfaces for the first two lowest electronic states of the Li (2p) + H₂ reaction. RSC Advances, 2018, 8, 15595-15602.	3.6	9
38	Investigations of Takeout proteinsâ€™ ligand binding and release mechanism using molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1464-1473.	3.5	3
39	Covalent surface modification with electron-donating/accepting Ï€-conjugated chains to effectively tune the electronic and magnetic properties of zigzag SiC nanoribbons. Journal of Materials Chemistry C, 2017, 5, 2022-2032.	5.5	7
40	Introducing the triangular BN nanodot or its cooperation with the edge-modification via the electron-donating/withdrawing group to achieve the large first hyperpolarizability in a carbon nanotube system. Physical Chemistry Chemical Physics, 2017, 19, 17834-17844.	2.8	13
41	Adsorbing the 3d-transition metal atoms to effectively modulate the electronic and magnetic behaviors of zigzag SiC nanoribbons. Physical Chemistry Chemical Physics, 2017, 19, 3694-3705.	2.8	9
42	Theoretical investigation on the interaction of hypergolic monomethylhydrazine with 1-chloro-1,1-dinitro-2-(N-chloroamidino)ethane using DFT methods. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	0
43	Accurate potential surfaces for the ground state of H+C2 reaction. European Physical Journal D, 2017, 71, 1.	1.3	7
44	Highly Active, Nonprecious Electrocatalyst Comprising Borophene Subunits for the Hydrogen Evolution Reaction. Journal of the American Chemical Society, 2017, 139, 12370-12373.	13.7	335
45	Second harmonic generation property of monolayer TMDCs and its potential application in producing terahertz radiation. Journal of Chemical Physics, 2017, 147, 244701.	3.0	19
46	Peculiar electronic, strong in-plane and out-of-plane second harmonic generation and piezoelectric properties of atom-thick Î±-M₂X₃ (M = Ga, In; X = S, Se): role of spontaneous electric dipole orientations. RSC Advances, 2017, 7, 55034-55043.	3.6	66
47	Unique Electronic Structure in a Porous Gaâ€In Bimetallic Oxide Nanoâ€Photocatalyst with Atomically Thin Pore Walls. Angewandte Chemie, 2016, 128, 11614-11618.	2.0	5
48	DFT study on the iridium-catalyzed multi-alkylation of alcohol with ammonia. RSC Advances, 2016, 6, 87362-87372.	3.6	6
49	Two sequential enhancements of laser-induced Cu plasma with cylindrical cavity confinement. Journal of Analytical Atomic Spectrometry, 2016, 31, 1974-1977.	3.0	25
50	Proximal environment controlling the reactivity between inorganic sulfide and heme-peptide model. RSC Advances, 2016, 6, 78858-78864.	3.6	11
51	Unique Electronic Structure in a Porous Gaâ€In Bimetallic Oxide Nanoâ€Photocatalyst with Atomically Thin Pore Walls. Angewandte Chemie - International Edition, 2016, 55, 11442-11446.	13.8	40
52	Structure advantage and peroxidase activity enhancement of deuterohemin-peptideâ€“inorganic hybrid flowers. RSC Advances, 2016, 6, 104265-104272.	3.6	22
53	Reaction mechanisms of methanol oxidation by <scp>Fe^{IV}O</scp> biomimetic complex. International Journal of Quantum Chemistry, 2016, 116, 692-701.	2.0	6
54	Immobilization of Lactobacillus rhamnosus in mesoporous silica-based material: An efficiency continuous cell-recycle fermentation system for lactic acid production. Journal of Bioscience and Bioengineering, 2016, 121, 645-651.	2.2	46

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55	Realizing diverse electronic and magnetic properties in hybrid zigzag BNC nanoribbons via hydrogenation. Physical Chemistry Chemical Physics, 2016, 18, 1326-1340.	2.8	9
56	Molecular simulations study of novel 1,4â€dihydropyridines derivatives with a high selectivity for <scp>C</scp>av3.1 calcium channel. Protein Science, 2015, 24, 1737-1747.	7.6	9
57	Ambipolar charge-transport properties in 4,10-dihalogenated anthanthrone crystals: a theoretical study. Journal of Materials Chemistry C, 2015, 3, 1913-1921.	5.5	8
58	Theoretical insights and design of intriguing nonlinear optical species involving the excess electron. International Journal of Quantum Chemistry, 2015, 115, 671-679.	2.0	41
59	Simulating the antimicrobial mechanism of human Î²-defensin-3 with coarse-grained molecular dynamics. Journal of Biomolecular Structure and Dynamics, 2015, 33, 2522-2529.	3.5	18
60	Theoretical insights into the reaction mechanism and solvation effect of conjugate addition of dimethyl propanedioate to 1-nitroprop-1-ene catalyzed by cinchona alkaloids. Structural Chemistry, 2015, 26, 951-959.	2.0	5
61	Hydrogen generation from alcohols (Î±-hydroxy carboxylic acids) and alcoholâ€“ammonia coupling in aqueous media catalysed by water-soluble bipyridine-Cp[*]Ir (Rh or Os) catalyst: a computational mechanism insight. Molecular Physics, 2015, 113, 1400-1412.	1.7	2
62	Molecular charge transfer via Ï€â€“Ï€ interaction: an effective approach to realize the half-metallicity and spin-gapless-semiconductor in zigzag graphene nanoribbon. RSC Advances, 2015, 5, 53003-53011.	3.6	11
63	Structures and nonlinear optical properties of lithium-adsorbed polycyclic Ï€-conjugated pentacene systems. Chemical Research in Chinese Universities, 2015, 31, 261-269.	2.6	3
64	Reactive scattering for Hâ¯â€‰+â€‰HD and Dâ¯â€‰+â€‰HD: classical trajectory investigation. European Physical Journal D, 2015, 69, 1.	1.3	3
65	Mechanistic study on the Cp*iridium-catalyzed N-alkylation of amines with alcohols. RSC Advances, 2015, 5, 22996-23008.	3.6	18
66	Conformational changes in MetNI: steered molecular dynamic studies of the methionine ABC transporter with and without substrates. Molecular Simulation, 2015, 41, 613-621.	2.0	1
67	Understanding the Effects of Bidentate Directing Groups: A Unified Rationale for sp2 and sp3 Câ€“H Bond Activations. Journal of Organic Chemistry, 2015, 80, 4672-4682.	3.2	58
68	DFT Study on the Homogeneous Palladium-Catalyzed N-Alkylation of Amines with Alcohols. ACS Catalysis, 2015, 5, 5728-5740.	11.2	26
69	Mechanistic studies on the pH-controllable interconversion between hydrogen and formic acid in water: DFT insights. New Journal of Chemistry, 2015, 39, 8060-8072.	2.8	5
70	Theoretical investigation on the reaction of HS+ with CH3NH2. Chemical Papers, 2014, 68, .	2.2	2
71	Theoretical investigation on mechanism of asymmetric Michael addition of trans-1-nitro-2-phenylethylene to 2-methylpropionaldehyde catalyzed by a Cinchona alkaloid-derived primary amine. Structural Chemistry, 2014, 25, 1343-1357.	2.0	5
72	Evaporation-induced morphology pattern of triblock copolymer A5B10C5 in thin film: A multibody DPD simulation study. Chemical Research in Chinese Universities, 2014, 30, 144-148.	2.6	3

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73	Dihalogen edge-modification: an effective approach to realize the half-metallicity and metallicity in zigzag silicon carbon nanoribbons. Journal of Materials Chemistry C, 2014, 2, 7836-7850.	5.5	28
74	A computational mechanistic study of pH-dependent alcohol dehydrogenation catalyzed by a novel [C,N] or [C,C] cyclometalated Cp*Ir complex in aqueous solution. New Journal of Chemistry, 2014, 38, 3862-3873.	2.8	9
75	Theoretical investigation on the mechanism of FeCl3-catalysed cross-coupling reaction of alcohols with alkenes. Molecular Physics, 2014, 112, 2107-2113.	1.7	1
76	Reactive scattering for Dâˆ’ + D2 (v = 0âˆ’1, j = 0âˆ’8): quantum and classical trajectory investigation. European Physical Journal D, 2014, 68, 1.	1.3	3
77	Effect of sample position on collinear femtosecond double-pulse laser-induced breakdown spectroscopy of silicon in air. Journal of Analytical Atomic Spectrometry, 2014, 29, 1105.	3.0	28
78	Theoretical investigation on nonlinear optical properties of carbon nanotubes with Stoneâ€“Wales defect rings. Journal of Materials Chemistry C, 2014, 2, 306-311.	5.5	42
79	Theoretical study on mechanism of cinchona alkaloids catalyzed asymmetric conjugate addition of dimethyl malonate to Î²-nitrostyrene. International Journal of Quantum Chemistry, 2014, 114, 642-651.	2.0	4
80	Theoretical studies on structures and stabilities of C4H2 + isomers. Chemical Research in Chinese Universities, 2013, 29, 150-153.	2.6	6
81	First principles investigation on the stability, magnetic and electronic properties of the fully and partially hydrogenated BN nanoribbons in different conformers. Journal of Materials Chemistry C, 2013, 1, 6890.	5.5	17
82	Reactive scattering for H+ + H2: non-Born-Oppenheimer classical investigation. European Physical Journal D, 2013, 67, 1.	1.3	1
83	An Effective Approach to Achieve a Spin Gapless Semiconductorâ€“Halfâ€Metalâ€“Metal Transition in Zigzag Graphene Nanoribbons: Attaching A Floating Induced Dipole Field via Ï€â€“Ï€ Interactions. Advanced Functional Materials, 2013, 23, 1507-1518.	14.9	37
84	The mechanism investigation of the imidazolidinone catalyzed fiveâ€membered ring synthesis reaction. Journal of Physical Organic Chemistry, 2013, 26, 232-239.	1.9	2
85	Constructing a mixed Ï€-conjugated bridge: a simple and effective approach to realize a large first hyperpolarizability in carbon nanotube-based systems. Journal of Materials Chemistry C, 2013, 1, 3833.	5.5	36
86	Graphene Nanoribbons: An Effective Approach to Achieve a Spin Gapless Semiconductorâ€“Halfâ€Metalâ€“Metal Transition in Zigzag Graphene Nanoribbons: Attaching A Floating Induced Dipole Field via Ï€â€“Ï€ Interactions (Adv. Funct. Mater. 12/2013). Advanced Functional Materials, 2013, 23, 1478-1478.	14.9	1
87	Theoretical investigation on structures, stability and properties of [P, X, Y] (X=C, Si; Yâ€‰=â€‰O, S) isomers. Molecular Physics, 2013, 111, 323-333.	1.7	6
88	Optimally enhanced optical emission in laser-induced air plasma by femtosecond double-pulse. Physics of Plasmas, 2013, 20, 103110.	1.9	28
89	POSITIONING OF Ftzâ€“F1 DOMAIN AFFECTS ON THE ACTIVITY OF HUMAN LRH-1: MOLECULAR DYNAMICS STUDY ON HUMAN LRH-1-DNA COMPLEXES. Journal of Theoretical and Computational Chemistry, 2012, 11, 329-359.	1.8	3
90	Aromatic Residues Regulating Electron Relay Ability of S-Containing Amino Acids by Formations of Sâˆ´Ï€ Multicenter Three-Electron Bonds in Proteins. Journal of Physical Chemistry C, 2012, 116, 19682-19688.	3.1	28

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91	Successive hydrogenation starting from the edge(s): an effective approach to fine-tune the electronic and magnetic behaviors of SiC nanoribbons. Journal of Materials Chemistry, 2012, 22, 24166.	6.7	32
92	Directab initiodynamics study of rate constants and kinetic isotope effects for C₂(A³Î_u)â€‰+â€‰CH₃OH reaction. Molecular Physics, 2012, 110, 2205-2217.	1.7	0
93	A theoretical study of the reaction of N(4 S) with nitrogen dioxide on the N2O2 potential energy surface. Russian Journal of Physical Chemistry A, 2012, 86, 1438-1446.	0.6	2
94	Theoretical study on the ionâ€“molecule reaction of NH⁺ with CH₂O. International Journal of Quantum Chemistry, 2012, 112, 1654-1666.	2.0	0
95	Direct ab initio dynamics study of the reaction of C₂(A³Î_u) with CH₄. International Journal of Quantum Chemistry, 2012, 112, 1078-1085.	2.0	10
96	3D hierarchical flower-like TiO2 nanostructure: morphology control and its photocatalytic property. CrystEngComm, 2011, 13, 2994.	2.6	237
97	Evaporation- and surface-induced morphology of symmetric diblock copolymer thin films: a multibody dissipative particle dynamics study. Molecular Simulation, 2011, 37, 875-883.	2.0	10
98	Theoretical study on the structures, isomerization and stability of SiC4 isomers. Theoretical Chemistry Accounts, 2010, 126, 15-25.	1.4	3
99	Structures and Stability of HNS2 Isomers. Chinese Journal of Chemistry, 2010, 20, 760-765.	4.9	2
100	Effect of substitution and cooperativity on the Clâ€“F blue shift in single-electron halogen-bonded H₃C Â·Â·Â· ClF complex. Molecular Physics, 2010, 108, 2021-2026.	1.7	11
101	AB INITIO INVESTIGATIONS OF THE RADICALâ€“RADICAL REACTION: N (4S) + NCO (X2Î). Journal of Theoretical and Computational Chemistry, 2009, 08, 587-595.	1.8	2
102	INTERACTIONS BETWEEN HUMAN SLINGSHOT PHOSPHATASE 2 AND PHOSPHO-COFILIN: A MOLECULAR DYNAMICS STUDY. Journal of Theoretical and Computational Chemistry, 2009, 08, 233-250.	1.8	1
103	Theoretical study on the reaction of CN radicals with ClO radicals by density functional theory. Science in China Series B: Chemistry, 2009, 52, 1973-1979.	0.8	0
104	Theoretical study on the mechanism of C2Cl3Â+ÂNO2 reaction. Theoretical Chemistry Accounts, 2009, 123, 431-441.	1.4	2
105	Radical reaction HCNOÂ+Â3NH: a mechanistic study. Theoretical Chemistry Accounts, 2009, 124, 123-137.	1.4	8
106	Theoretical study on the ionâ€“molecule reaction of HCN+ with NH3. Theoretical Chemistry Accounts, 2009, 124, 409-420.	1.4	1
107	Bonding and correlation analysis of various Si₂CO isomers on the potential energy surface. International Journal of Quantum Chemistry, 2009, 109, 907-919.	2.0	0
108	Direct dynamic study on the hydrogen abstraction reaction of H₂CO with NCO. International Journal of Chemical Kinetics, 2009, 41, 394-400.	1.6	1

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109	Band-Gap-Controllable Photonic Crystals Consisting of Magnetic Nanocrystal Clusters in a Solidified Polymer Matrix. Journal of Physical Chemistry C, 2009, 113, 18542-18545.	3.1	30
110	A barrierâ€free atomic radicalâ€molecule reaction: N (²D) NO₂ (²A₁) mechanistic study. International Journal of Quantum Chemistry, 2008, 108, 1309-1315.	2.0	2
111	The adsorption of poly (vinyl alcohol) on the hydroxylated Î²-cristobalite. Molecular Simulation, 2008, 34, 611-618.	2.0	2
112	Theoretical study of the [Si, C, P, O] potential energy surface. Molecular Physics, 2007, 105, 2423-2432.	1.7	1
113	Theoretical Elucidation of the Platinum-Mediated Arene Câ^'H Activation Reactions. Organometallics, 2007, 26, 2203-2210.	2.3	16
114	Theoretical study of the Si2NO potential energy surface. International Journal of Quantum Chemistry, 2007, 107, 1181-1193.	2.0	2
115	Atomic radicalâ€"molecule reactions F +Â CH3Câ‰¡CH: mechanistic study. Theoretical Chemistry Accounts, 2007, 117, 417-429.	1.4	4
116	Theoretical study on the potential energy surface of NC3P isomers. Theoretical Chemistry Accounts, 2007, 117, 501-520.	1.4	0
117	A barrier-free molecular radical-molecule reaction: $${^{3}C_{2} (a^{3}Pi) {+} O_{2} (X^{3}) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.4	3
118	Theoretical study on structures and stability of triplet SiC3O isomers. Theoretical Chemistry Accounts, 2007, 118, 383-397.	1.4	0
119	Theoretical study on the potential energy surface of NC3P isomers. Theoretical Chemistry Accounts, 2007, 118, 739-754.	1.4	1
120	A CASPT2//CASSCF study of the quartet excited state $$ilde{a}^{4}A^{primeprime}$$ of the HCNN radical. Theoretical Chemistry Accounts, 2007, 118, 915-922.	1.4	2
121	A Barrier-Free Atomic Radical-Molecule Reaction:â€‰ F + Propene. Journal of Chemical Theory and Computation, 2006, 2, 1551-1564.	5.3	19
122	Structure and Stability of Isomers of the Promising Interstellar Molecule PC3O. Theoretical Chemistry Accounts, 2006, 115, 410-426.	1.4	2
123	SiC3N:â€‰ A Promising Interstellar Molecule with Stable Cyclic Isomers. Journal of Physical Chemistry A, 2004, 108, 6919-6927.	2.5	15
124	A Theoretical Study on the Potential Energy Surface of the 3C2 + NO Reaction. Journal of Physical Chemistry A, 2004, 108, 6771-6777.	2.5	5
125	Theoretical Mechanistic Study on the Ionâ^'Molecule Reactions of CCN+/CNC+with H2S. Journal of Physical Chemistry A, 2002, 106, 2949-2962.	2.5	5
126	Theoretical study of the hydrogen abstraction by chlorine atoms for CH2BrCl and CHBrCl2. Physical Chemistry Chemical Physics, 2002, 4, 46-50.	2.8	4

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127	Theoretical study on mechanisms of the high-temperature reactions C2H3â€‰+â€‰H2O and C2H4â€‰+â€‰OHElectronic supplementary information (ESI) available: Figures of optimized geometries of the fragments of C2H5O radicals, C2H5O isomers and C2H5O transition states and table of harmonic vibration frequencies of C2H3, H2O, TSR/P1, C2H4 and OH. See http://www.rsc.org/suppdata/cp/b1/b109758j/. Physical Chemistry Chemical Physics, 2002, 4, 1021-1027.	2.8	27
128	Direct ab initio dynamics calculations of the reaction rates for the hydrogen abstraction reaction Clâ€‰+â€‰HC(O)Fâ€‰â†’â€‰HClâ€‰+â€‰CFO. Physical Chemistry Chemical Physics, 2002, 4, 2927-2931.	2.8	3
129	Theoretical mechanistic study on the ionâ€“molecule reactions of CCN+/CNC+ with H2O and HCO+/HOC+ with HCN/HNC. Journal of Chemical Physics, 2002, 116, 1892-1910.	3.0	2
130	Theoretical study on structures and stability of HC2P isomers. Theoretical Chemistry Accounts, 2002, 107, 253-265.	1.4	11
131	Direct ab initio dynamics calculations on the rate constants for the hydrogen-abstraction reaction of C 2 H 5 F with O (3 P). Theoretical Chemistry Accounts, 2002, 108, 179-186.	1.4	3
132	Structure and Stability of Interstellar Molecule C₃S. Chinese Journal of Chemistry, 2002, 20, 1487-1493.	4.9	4
133	C4N: The first CnN radical with stable cyclic isomers. Journal of Chemical Physics, 2001, 114, 5170-5179.	3.0	18
134	Theoretical Study on Potential Energy Surface of the Interstellar Molecule SiC2N. Journal of Physical Chemistry A, 2001, 105, 5896-5901.	2.5	23
135	Theoretical Study on Reaction Mechanism of the Methylidyne Radical with Nitrogen Dioxide. Journal of Physical Chemistry A, 2001, 105, 3388-3399.	2.5	16
136	Theoretical study of the potential-energy surface of C 2 NP. Theoretical Chemistry Accounts, 2001, 107, 1-7.	1.4	3
137	Theoretical study on reaction mechanism of the CF radical with nitrogen dioxide. Journal of Computational Chemistry, 2001, 22, 1907-1919.	3.3	6
138	CCNN: The last kinetically stable isomer of cyanogen. Journal of Chemical Physics, 2000, 113, 1745-1754.	3.0	22
139	Curing theory of A f -A g type free radical polymerization (II). Science in China Series B: Chemistry, 1999, 42, 14-19.	0.8	2
140	Molecular dynamics simulation of polystyrene-block-poly(methyl methacrylate). Macromolecular Theory and Simulations, 1998, 7, 619-622.	1.4	2
141	Tree-gel and loop-gel conversions in nonlinear polymerization. Science in China Series B: Chemistry, 1998, 41, 122-134.	0.8	2
142	Curing theory of A f -A g type free radical polymerization (I). Science in China Series B: Chemistry, 1998, 41, 652-659.	0.8	1
143	The sol fraction and conversions in AaBb type polymerisation. Macromolecular Theory and Simulations, 1995, 4, 1055-1061.	1.4	0