

Xu-ri Huang

List of Publications by Year in descending order

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143
papers

2,252
citations

304743

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all docs

143
docs citations

143
times ranked

3470
citing authors

#	ARTICLE	IF	CITATIONS
1	Highly Active, Nonprecious Electrocatalyst Comprising Borophene Subunits for the Hydrogen Evolution Reaction. <i>Journal of the American Chemical Society</i> , 2017, 139, 12370-12373.	13.7	335
2	Efficient oxygen evolution electrocatalysis in acid by a perovskite with face-sharing IrO ₆ octahedral dimers. <i>Nature Communications</i> , 2018, 9, 5236.	12.8	325
3	3D hierarchical flower-like TiO ₂ nanostructure: morphology control and its photocatalytic property. <i>CrystEngComm</i> , 2011, 13, 2994.	2.6	237
4	Peculiar electronic, strong in-plane and out-of-plane second harmonic generation and piezoelectric properties of atom-thick $1\pm$ -M ₂ X ₃ (M = Ga, In; X = S, Se): role of spontaneous electric dipole orientations. <i>RSC Advances</i> , 2017, 7, 55034-55043.	3.6	66
5	Understanding the Effects of Bidentate Directing Groups: A Unified Rationale for sp ² and sp ³ C-H Bond Activations. <i>Journal of Organic Chemistry</i> , 2015, 80, 4672-4682.	3.2	58
6	Immobilization of <i>Lactobacillus rhamnosus</i> in mesoporous silica-based material: An efficiency continuous cell-recycle fermentation system for lactic acid production. <i>Journal of Bioscience and Bioengineering</i> , 2016, 121, 645-651.	2.2	46
7	Theoretical investigation on nonlinear optical properties of carbon nanotubes with Stone-Wales defect rings. <i>Journal of Materials Chemistry C</i> , 2014, 2, 306-311.	5.5	42
8	Theoretical insights and design of intriguing nonlinear optical species involving the excess electron. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 671-679.	2.0	41
9	Unique Electronic Structure in a Porous Ga-In Bimetallic Oxide Nano-Photocatalyst with Atomically Thin Pore Walls. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 11442-11446.	13.8	40
10	Metal-ionic-conductor potassium ferrite nanocrystals with intrinsic superhydrophilic surfaces for electrocatalytic water splitting at ultrahigh current densities. <i>Journal of Materials Chemistry A</i> , 2021, 9, 7586-7593.	10.3	40
11	An Effective Approach to Achieve a Spin Gapless Semiconductor-Half-Metal-Metal Transition in Zigzag Graphene Nanoribbons: Attaching A Floating Induced Dipole Field via π - π Interactions. <i>Advanced Functional Materials</i> , 2013, 23, 1507-1518.	14.9	37
12	Constructing a mixed π -conjugated bridge: a simple and effective approach to realize a large first hyperpolarizability in carbon nanotube-based systems. <i>Journal of Materials Chemistry C</i> , 2013, 1, 3833.	5.5	36
13	Successive hydrogenation starting from the edge(s): an effective approach to fine-tune the electronic and magnetic behaviors of SiC nanoribbons. <i>Journal of Materials Chemistry</i> , 2012, 22, 24166.	6.7	32
14	Band-Gap-Controllable Photonic Crystals Consisting of Magnetic Nanocrystal Clusters in a Solidified Polymer Matrix. <i>Journal of Physical Chemistry C</i> , 2009, 113, 18542-18545.	3.1	30
15	Aromatic Residues Regulating Electron Relay Ability of S-Containing Amino Acids by Formations of S π - π Multicenter Three-Electron Bonds in Proteins. <i>Journal of Physical Chemistry C</i> , 2012, 116, 19682-19688.	3.1	28
16	Optimally enhanced optical emission in laser-induced air plasma by femtosecond double-pulse. <i>Physics of Plasmas</i> , 2013, 20, 103110.	1.9	28
17	Dihalogen edge-modification: an effective approach to realize the half-metallicity and metallicity in zigzag silicon carbon nanoribbons. <i>Journal of Materials Chemistry C</i> , 2014, 2, 7836-7850.	5.5	28
18	Effect of sample position on collinear femtosecond double-pulse laser-induced breakdown spectroscopy of silicon in air. <i>Journal of Analytical Atomic Spectrometry</i> , 2014, 29, 1105.	3.0	28

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19	Theoretical study on mechanisms of the high-temperature reactions $C_2H_3 + H_2O$ and $C_2H_4 + OH$. Electronic supplementary information (ESI) available: Figures of optimized geometries of the fragments of C_2H_5O radicals, C_2H_5O isomers and C_2H_5O transition states and table of harmonic vibration frequencies of C_2H_3 , H_2O , $TSR/P1$, C_2H_4 and OH . See http://www.rsc.org/suppdata/cpl/b1/b100758j/ . <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 1021-1027.	2.8	27
20	DFT Study on the Homogeneous Palladium-Catalyzed N-Alkylation of Amines with Alcohols. <i>ACS Catalysis</i> , 2015, 5, 5728-5740.	11.2	26
21	Two sequential enhancements of laser-induced Cu plasma with cylindrical cavity confinement. <i>Journal of Analytical Atomic Spectrometry</i> , 2016, 31, 1974-1977.	3.0	25
22	Theoretical Study on Potential Energy Surface of the Interstellar Molecule SiC_2N . <i>Journal of Physical Chemistry A</i> , 2001, 105, 5896-5901.	2.5	23
23	CCNN: The last kinetically stable isomer of cyanogen. <i>Journal of Chemical Physics</i> , 2000, 113, 1745-1754.	3.0	22
24	Structure advantage and peroxidase activity enhancement of deuterohemin-peptide-inorganic hybrid flowers. <i>RSC Advances</i> , 2016, 6, 104265-104272.	3.6	22
25	Applying surface strain and coupling with pure or N/B-doped graphene to successfully achieve high HER catalytic activity in 2D layered SnP_3 -based nanomaterials: a first-principles investigation. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 647-658.	6.0	22
26	Embedding tetrahedral 3d transition metal TM_4 clusters into the cavity of two-dimensional graphdiyne to construct highly efficient and nonprecious electrocatalysts for hydrogen evolution reaction. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 3254-3263.	2.8	20
27	A Barrier-Free Atomic Radical-Molecule Reaction: $F + Propene$. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1551-1564.	5.3	19
28	Second harmonic generation property of monolayer TMDCs and its potential application in producing terahertz radiation. <i>Journal of Chemical Physics</i> , 2017, 147, 244701.	3.0	19
29	C_4N : The first C_nN radical with stable cyclic isomers. <i>Journal of Chemical Physics</i> , 2001, 114, 5170-5179.	3.0	18
30	Simulating the antimicrobial mechanism of human β -defensin-3 with coarse-grained molecular dynamics. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 2522-2529.	3.5	18
31	Mechanistic study on the Cp^* iridium-catalyzed N-alkylation of amines with alcohols. <i>RSC Advances</i> , 2015, 5, 22996-23008.	3.6	18
32	First principles investigation on the stability, magnetic and electronic properties of the fully and partially hydrogenated BN nanoribbons in different conformers. <i>Journal of Materials Chemistry C</i> , 2013, 1, 6890.	5.5	17
33	Host-Guest Interaction Creates Hydrogen-Evolution Electrocatalytic Active Sites in 3d Transition Metal-Intercalated Titanates. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 696-703.	8.0	17
34	Theoretical Study on Reaction Mechanism of the Methylidyne Radical with Nitrogen Dioxide. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3388-3399.	2.5	16
35	Theoretical Elucidation of the Platinum-Mediated Arene $C-H$ Activation Reactions. <i>Organometallics</i> , 2007, 26, 2203-2210.	2.3	16
36	SiC_3N : A Promising Interstellar Molecule with Stable Cyclic Isomers. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6919-6927.	2.5	15

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37	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. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17834-17844.	2.8	13
38	Theoretical study on structures and stability of HC ₂ P isomers. <i>Theoretical Chemistry Accounts</i> , 2002, 107, 253-265.	1.4	11
39	Effect of substitution and cooperativity on the Cl ⁻ F blue shift in single-electron halogen-bonded H ₃ C ··· ClF complex. <i>Molecular Physics</i> , 2010, 108, 2021-2026.	1.7	11
40	Molecular charge transfer via π - π interaction: an effective approach to realize the half-metallicity and spin-gapless-semiconductor in zigzag graphene nanoribbon. <i>RSC Advances</i> , 2015, 5, 53003-53011.	3.6	11
41	Proximal environment controlling the reactivity between inorganic sulfide and heme-peptide model. <i>RSC Advances</i> , 2016, 6, 78858-78864.	3.6	11
42	Probing the activity of transition metal M and heteroatom N ₄ co-doped in vacancy fullerene (M@N ₄ @C ₆₄ , M = Fe, Co, and Ni) towards the oxygen reduction reaction by density functional theory. <i>RSC Advances</i> , 2021, 11, 3174-3182.	3.6	11
43	Evaporation- and surface-induced morphology of symmetric diblock copolymer thin films: a multibody dissipative particle dynamics study. <i>Molecular Simulation</i> , 2011, 37, 875-883.	2.0	10
44	Direct ab initio dynamics study of the reaction of C ₂ (A ³⁺ ⋯) with CH ₄ . <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1078-1085.	2.0	10
45	Methanol activation catalyzed by Pt ₇ , Pt ₃ Cu ₄ , and Cu ₇ clusters: A density functional theory investigation. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4197.	3.5	10
46	Reaction of CO ₂ with Atomic Transition Metal M ^{+/0} Ions: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5848-5860.	2.5	10
47	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. <i>New Journal of Chemistry</i> , 2014, 38, 3862-3873.	2.8	9
48	Molecular simulations study of novel 1,4-dihydropyridines derivatives with a high selectivity for Ca^{2+} calcium channel. <i>Protein Science</i> , 2015, 24, 1737-1747.	7.6	9
49	Realizing diverse electronic and magnetic properties in hybrid zigzag BNC nanoribbons via hydrogenation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1326-1340.	2.8	9
50	Adsorbing the 3d-transition metal atoms to effectively modulate the electronic and magnetic behaviors of zigzag SiC nanoribbons. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3694-3705.	2.8	9
51	Accurate potential energy surfaces for the first two lowest electronic states of the Li (2p) + H ₂ reaction. <i>RSC Advances</i> , 2018, 8, 15595-15602.	3.6	9
52	Theoretical Study on a Potential Oxygen Reduction Reaction Electrocatalyst: Single Fe Atoms Supported on Graphite Carbonitride. <i>Langmuir</i> , 2021, 37, 428-436.	3.5	9
53	Radical reaction HCNO + NH ₃ : a mechanistic study. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 123-137.	1.4	8
54	Ambipolar charge-transport properties in 4,10-dihalogenated anthanthrone crystals: a theoretical study. <i>Journal of Materials Chemistry C</i> , 2015, 3, 1913-1921.	5.5	8

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55	Covalent surface modification with electron-donating/accepting π -conjugated chains to effectively tune the electronic and magnetic properties of zigzag SiC nanoribbons. <i>Journal of Materials Chemistry C</i> , 2017, 5, 2022-2032.	5.5	7
56	Accurate potential surfaces for the ground state of H+C ₂ reaction. <i>European Physical Journal D</i> , 2017, 71, 1.	1.3	7
57	An accurate ground state potential surface for the scattering reaction $F^{2+} + F_2 \rightarrow F^{2+} + F_2$. <i>RSC Advances</i> , 2019, 9, 1929-1932.	2.1	7
58	Realizing Efficient Catalytic Performance and High Selectivity for Oxygen Reduction Reaction on a 2D Ni ₂ SbTe ₂ Monolayer. <i>Inorganic Chemistry</i> , 2022, 61, 2284-2291.	4.0	7
59	Theoretical study on reaction mechanism of the CF radical with nitrogen dioxide. <i>Journal of Computational Chemistry</i> , 2001, 22, 1907-1919.	3.3	6
60	Theoretical studies on structures and stabilities of C ₄ H ₂ + isomers. <i>Chemical Research in Chinese Universities</i> , 2013, 29, 150-153.	2.6	6
61	Theoretical investigation on structures, stability and properties of [P, X, Y] (X=C, Si; Y=O, S) isomers. <i>Molecular Physics</i> , 2013, 111, 323-333.	1.7	6
62	DFT study on the iridium-catalyzed multi-alkylation of alcohol with ammonia. <i>RSC Advances</i> , 2016, 6, 87362-87372.	3.6	6
63	Reaction mechanisms of methanol oxidation by $Fe^{IV}O$ biomimetic complex. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 692-701.	2.0	6
64	Adsorbing the magnetic superhalogen MnCl ₃ to realize intriguing half-metallic and spin-gapless-semiconducting behavior in zigzag or armchair SiC nanoribbon. <i>RSC Advances</i> , 2018, 8, 13167-13177.	3.6	6
65	Theoretical Mechanistic Study on the Ion-Molecule Reactions of CCN ⁺ /CNC ⁺ with H ₂ S. <i>Journal of Physical Chemistry A</i> , 2002, 106, 2949-2962.	2.5	5
66	A Theoretical Study on the Potential Energy Surface of the 3C ₂ + NO Reaction. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6771-6777.	2.5	5
67	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. <i>Structural Chemistry</i> , 2014, 25, 1343-1357.	2.0	5
68	Theoretical insights into the reaction mechanism and solvation effect of conjugate addition of dimethyl propanedioate to 1-nitroprop-1-ene catalyzed by cinchona alkaloids. <i>Structural Chemistry</i> , 2015, 26, 951-959.	2.0	5
69	Mechanistic studies on the pH-controllable interconversion between hydrogen and formic acid in water: DFT insights. <i>New Journal of Chemistry</i> , 2015, 39, 8060-8072.	2.8	5
70	Unique Electronic Structure in a Porous GaIn Bimetallic Oxide Nano-Photocatalyst with Atomically Thin Pore Walls. <i>Angewandte Chemie</i> , 2016, 128, 11614-11618.	2.0	5
71	Methanol dissociation and oxidation on single Fe atom supported on graphitic carbon nitride. <i>Applied Organometallic Chemistry</i> , 2019, 33, e4930.	3.5	5
72	Theoretical study of substituent effects on electride characteristics and the nonlinear optical properties of Li@calix[4]pyrrole. <i>RSC Advances</i> , 2019, 9, 37919-37925.	3.6	5

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73	Molecular dynamics simulations investigate the pathway of substrate entry active site of rhomboid protease. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 3445-3455.	3.5	5
74	Global accurate diabatic potential surfaces for the reaction $H + Li_2$. <i>RSC Advances</i> , 2020, 10, 39226-39240.	3.6	5
75	Activity adaptability of a DhHP-6 peroxidase-mimic in wide pH and temperature ranges and solvent media. <i>Catalysis Science and Technology</i> , 2020, 10, 1848-1857.	4.1	5
76	Theoretical study of the hydrogen abstraction by chlorine atoms for CH_2BrCl and $CHBrCl_2$. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 46-50.	2.8	4
77	Atomic radical molecule reactions $F + CH_3C\dot{C}H$: mechanistic study. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 417-429.	1.4	4
78	Structure and Stability of Interstellar Molecule C_3S . <i>Chinese Journal of Chemistry</i> , 2002, 20, 1487-1493.	4.9	4
79	Theoretical study on mechanism of cinchona alkaloids catalyzed asymmetric conjugate addition of dimethyl malonate to β -nitrostyrene. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 642-651.	2.0	4
80	Theoretical study of the potential-energy surface of C_2 NP. <i>Theoretical Chemistry Accounts</i> , 2001, 107, 1-7.	1.4	3
81	Direct ab initio dynamics calculations of the reaction rates for the hydrogen abstraction reaction $Cl + HC(O)F + HCl + CFO$. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 2927-2931.	2.8	3
82	Direct ab initio dynamics calculations on the rate constants for the hydrogen-abstraction reaction of C_2H_5F with $O(3P)$. <i>Theoretical Chemistry Accounts</i> , 2002, 108, 179-186.	1.4	3
83	A barrier-free molecular radical-molecule reaction: $C_2(a^3\Pi) + O_2(X^3\Sigma^-_g)$. <i>Journal of Chemical Physics</i> , 2014, 140, 174301.	1.4	3
84	Theoretical study on the structures, isomerization and stability of SiC_4 isomers. <i>Theoretical Chemistry Accounts</i> , 2010, 126, 15-25.	1.4	3
85	POSITIONING OF F1 DOMAIN AFFECTS ON THE ACTIVITY OF HUMAN LRH-1: MOLECULAR DYNAMICS STUDY ON HUMAN LRH-1-DNA COMPLEXES. <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 329-359.	1.8	3
86	Evaporation-induced morphology pattern of triblock copolymer A5B10C5 in thin film: A multibody DPD simulation study. <i>Chemical Research in Chinese Universities</i> , 2014, 30, 144-148.	2.6	3
87	Reactive scattering for $D^+ + D_2(v=0, j=8)$: quantum and classical trajectory investigation. <i>European Physical Journal D</i> , 2014, 68, 1.	1.3	3
88	Structures and nonlinear optical properties of lithium-adsorbed polycyclic π -conjugated pentacene systems. <i>Chemical Research in Chinese Universities</i> , 2015, 31, 261-269.	2.6	3
89	Reactive scattering for $H^+ + HD$ and $D^+ + HD$: classical trajectory investigation. <i>European Physical Journal D</i> , 2015, 69, 1.	1.3	3
90	Investigations of Takeout proteins™ ligand binding and release mechanism using molecular dynamics simulation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017, 35, 1464-1473.	3.5	3

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91	Dissociation and oxidation mechanism of methanol on Al ₁₂ N ₁₂ cage: a DFT study. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	1.4	3
92	Theoretical investigation on the structures, electronic and magnetic properties of new 2D/1D composite nanosystems by adsorbing superhalogen MnCl ₃ on the BN monolayer/nanoribbons. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	1.4	3
93	Theoretical study of a novel organic electride with large nonlinear optical responses. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26235.	2.0	3
94	Heteroatom-doped fullerene C ₇₀ as non-metal electrocatalysts for oxygen reduction and oxygen evolution from computational study. <i>Diamond and Related Materials</i> , 2022, 124, 108954.	3.9	3
95	Molecular dynamics simulation of polystyrene-block-poly(methyl methacrylate). <i>Macromolecular Theory and Simulations</i> , 1998, 7, 619-622.	1.4	2
96	Tree-gel and loop-gel conversions in nonlinear polymerization. <i>Science in China Series B: Chemistry</i> , 1998, 41, 122-134.	0.8	2
97	Curing theory of A f -A g type free radical polymerization (II). <i>Science in China Series B: Chemistry</i> , 1999, 42, 14-19.	0.8	2
98	Theoretical mechanistic study on the ion-molecule reactions of CCN ⁺ /CNC ⁺ with H ₂ O and HCO ⁺ /HOC ⁺ with HCN/HNC. <i>Journal of Chemical Physics</i> , 2002, 116, 1892-1910.	3.0	2
99	Structure and Stability of Isomers of the Promising Interstellar Molecule PC ₃ O. <i>Theoretical Chemistry Accounts</i> , 2006, 115, 410-426.	1.4	2
100	Theoretical study of the Si ₂ NO potential energy surface. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1181-1193.	2.0	2
101	A CASPT2//CASSCF study of the quartet excited state $\tilde{a}^4A^{\prime\prime}$ of the HCNN radical. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 915-922.	1.4	2
102	A barrier-free atomic radical-molecule reaction: N(² D) NO(²) (² A ₁) mechanistic study. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1309-1315.	2.0	2
103	The adsorption of poly (vinyl alcohol) on the hydroxylated β -cristobalite. <i>Molecular Simulation</i> , 2008, 34, 611-618.	2.0	2
104	AB INITIO INVESTIGATIONS OF THE RADICAL-RADICAL REACTION: N (4S) + NCO (X ² $\tilde{1}$). <i>Journal of Theoretical and Computational Chemistry</i> , 2009, 08, 587-595.	1.8	2
105	Theoretical study on the mechanism of C ₂ Cl ₃ +NO ₂ reaction. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 431-441.	1.4	2
106	Structures and Stability of HNS ₂ Isomers. <i>Chinese Journal of Chemistry</i> , 2010, 20, 760-765.	4.9	2
107	A theoretical study of the reaction of N(4 S) with nitrogen dioxide on the N ₂ O ₂ potential energy surface. <i>Russian Journal of Physical Chemistry A</i> , 2012, 86, 1438-1446.	0.6	2
108	The mechanism investigation of the imidazolidinone catalyzed five-membered ring synthesis reaction. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 232-239.	1.9	2

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109	Theoretical investigation on the reaction of HS ⁺ with CH ₃ NH ₂ . Chemical Papers, 2014, 68, .	2.2	2
110	Hydrogen generation from alcohols (<i>α</i> -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
111	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
112	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
113	Catalytic activity of Ru ₄ -doped vacancy fullerenes (Ru ₄ @C ₅₄) theory investigation. Applied Organometallic Chemistry, 2022, 36, .	3.5	2
114	Generation of singlet oxygen catalyzed by the room-temperature-stable anthraquinone anion radical. Physical Chemistry Chemical Physics, 2022, 24, 14165-14171.	2.8	2
115	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
116	Theoretical study of the [Si, C, P, O] potential energy surface. Molecular Physics, 2007, 105, 2423-2432.	1.7	1
117	Theoretical study on the potential energy surface of NC ₃ P isomers. Theoretical Chemistry Accounts, 2007, 118, 739-754.	1.4	1
118	INTERACTIONS BETWEEN HUMAN SLINGSHOT PHOSPHATASE 2 AND PHOSPHO-COFLIN: A MOLECULAR DYNAMICS STUDY. Journal of Theoretical and Computational Chemistry, 2009, 08, 233-250.	1.8	1
119	Theoretical study on the ionâ€‘molecule reaction of HCN ⁺ with NH ₃ . Theoretical Chemistry Accounts, 2009, 124, 409-420.	1.4	1
120	Direct dynamic study on the hydrogen abstraction reaction of H ₂ CO with NCO. International Journal of Chemical Kinetics, 2009, 41, 394-400.	1.6	1
121	Reactive scattering for H ⁺ + H ₂ : non-Born-Oppenheimer classical investigation. European Physical Journal D, 2013, 67, 1.	1.3	1
122	Graphene Nanoribbons: An Effective Approach to Achieve a Spin Gapless Semiconductorâ€‘Halfâ€‘Metal Transition in Zigzag Graphene Nanoribbons: Attaching A Floating Induced Dipole Field via π - π Interactions (Adv. Funct. Mater. 12/2013). Advanced Functional Materials, 2013, 23, 1478-1478.	14.9	1
123	Theoretical investigation on the mechanism of FeCl ₃ -catalysed cross-coupling reaction of alcohols with alkenes. Molecular Physics, 2014, 112, 2107-2113.	1.7	1
124	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
125	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
126	Conformational transitions of uracil transporter UraA from <i>Escherichia coli</i> : a molecular simulation study. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3398-3410.	3.5	1

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