Xu-ri Huang

List of Publications by Year
in descending order

143	2,252	304368	253896
papers	citations	22 h-index	43 g-index

143	143	143	3470
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Highly Active, Nonprecious Electrocatalyst Comprising Borophene Subunits for the Hydrogen Evolution Reaction. Journal of the American Chemical Society, 2017, 139, 12370-12373.	6.6	335
2	Efficient oxygen evolution electrocatalysis in acid by a perovskite with face-sharing IrO6 octahedral dimers. Nature Communications, 2018, 9, 5236.	5.8	325
3	3D hierarchical flower-like TiO2 nanostructure: morphology control and its photocatalytic property. CrystEngComm, 2011, 13, 2994.	1.3	237
4	Peculiar electronic, strong in-plane and out-of-plane second harmonic generation and piezoelectric properties of atom-thick Ì±-M₂X₃ (M = Ga, In; X = S, Se): role of spontaneous electric dipole orientations. RSC Advances, 2017, 7, 55034-55043.	1.7	66
5	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.	1.7	58
6	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.	1.1	46
7	Theoretical investigation on nonlinear optical properties of carbon nanotubes with Stoneâ€“Wales defect rings. Journal of Materials Chemistry C, 2014, 2, 306-311.	2.7	42
8	Theoretical insights and design of intriguing nonlinear optical species involving the excess electron. International Journal of Quantum Chemistry, 2015, 115, 671-679.	1.0	41
9	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.	7.2	40
10	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.	5.2	40
11	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.	7.8	37
12	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.	2.7	36
13	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
14	Band-Gap-Controllable Photonic Crystals Consisting of Magnetic Nanocrystal Clusters in a Solidified Polymer Matrix. Journal of Physical Chemistry C, 2009, 113, 18542-18545.	1.5	30
15	Aromatic Residues Regulating Electron Relay Ability of S-Containing Amino Acids by Formations of Sâ^Ï€ Multicenter Three-Electron Bonds in Proteins. Journal of Physical Chemistry C, 2012, 116, 19682-19688.	1.5	28
16	Optimally enhanced optical emission in laser-induced air plasma by femtosecond double-pulse. Physics of Plasmas, 2013, 20, 103110.	0.7	28
17	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.	2.7	28
18	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.	1.6	28

#	Article	IF	Citations
19	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.	1.3	27
20	DFT Study on the Homogeneous Palladium-Catalyzed N-Alkylation of Amines with Alcohols. ACS Catalysis, 2015, 5, 5728-5740.	5.5	26
21	Two sequential enhancements of laser-induced Cu plasma with cylindrical cavity confinement. Journal of Analytical Atomic Spectrometry, 2016, 31, 1974-1977.	1.6	25
22	Theoretical Study on Potential Energy Surface of the Interstellar Molecule SiC2N. Journal of Physical Chemistry A, 2001, 105, 5896-5901.	1.1	23
23	CCNN: The last kinetically stable isomer of cyanogen. Journal of Chemical Physics, 2000, 113, 1745-1754.	1.2	22
24	Structure advantage and peroxidase activity enhancement of deuterohemin-peptideâ€“inorganic hybrid flowers. RSC Advances, 2016, 6, 104265-104272.	1.7	22
25	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.	3.0	22
26	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.	1.3	20
27	A Barrier-Free Atomic Radical-Molecule Reaction:â€‰ F + Propene. Journal of Chemical Theory and Computation, 2006, 2, 1551-1564.	2.3	19
28	Second harmonic generation property of monolayer TMDCs and its potential application in producing terahertz radiation. Journal of Chemical Physics, 2017, 147, 244701.	1.2	19
29	C4N: The first CnN radical with stable cyclic isomers. Journal of Chemical Physics, 2001, 114, 5170-5179.	1.2	18
30	Simulating the antimicrobial mechanism of human Î²-defensin-3 with coarse-grained molecular dynamics. Journal of Biomolecular Structure and Dynamics, 2015, 33, 2522-2529.	2.0	18
31	Mechanistic study on the Cp*iridium-catalyzed N-alkylation of amines with alcohols. RSC Advances, 2015, 5, 22996-23008.	1.7	18
32	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.	2.7	17
33	Hostâ€“Guest Interaction Creates Hydrogen-Evolution Electrocatalytic Active Sites in 3d Transition Metal-Intercalated Titanates. ACS Applied Materials & Interfaces, 2018, 10, 696-703.	4.0	17
34	Theoretical Study on Reaction Mechanism of the Methylidyne Radical with Nitrogen Dioxide. Journal of Physical Chemistry A, 2001, 105, 3388-3399.	1.1	16
35	Theoretical Elucidation of the Platinum-Mediated Arene Câˆ’H Activation Reactions. Organometallics, 2007, 26, 2203-2210.	1.1	16
36	SiC3N:â€‰ A Promising Interstellar Molecule with Stable Cyclic Isomers. Journal of Physical Chemistry A, 2004, 108, 6919-6927.	1.1	15

#	Article	IF	Citations
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. Physical Chemistry Chemical Physics, 2017, 19, 17834-17844.	1.3	13
38	Theoretical study on structures and stability of HC2P isomers. Theoretical Chemistry Accounts, 2002, 107, 253-265.	0.5	11
39	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.	0.8	11
40	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.	1.7	11
41	Proximal environment controlling the reactivity between inorganic sulfide and heme-peptide model. RSC Advances, 2016, 6, 78858-78864.	1.7	11
42	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.	1.7	11
43	Evaporation- and surface-induced morphology of symmetric diblock copolymer thin films: a multibody dissipative particle dynamics study. Molecular Simulation, 2011, 37, 875-883.	0.9	10
44	Direct ab initio dynamics study of the reaction of C₂(A³Î_u) with CH₄. International Journal of Quantum Chemistry, 2012, 112, 1078-1085.	1.0	10
45	Methanol activation catalyzed by Pt₇, Pt₃Cu₄, and Cu₇ clusters: A density functional theory investigation. Applied Organometallic Chemistry, 2018, 32, e4197.	1.7	10
46	Reaction of CO₂ with Atomic Transition Metal M^{+/0/â€“} Ions: A Theoretical Study. Journal of Physical Chemistry A, 2018, 122, 5848-5860.	1.1	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. New Journal of Chemistry, 2014, 38, 3862-3873.	1.4	9
48	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.	3.1	9
49	Realizing diverse electronic and magnetic properties in hybrid zigzag BNC nanoribbons via hydrogenation. Physical Chemistry Chemical Physics, 2016, 18, 1326-1340.	1.3	9
50	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.	1.3	9
51	Accurate potential energy surfaces for the first two lowest electronic states of the Li (2p) + H₂ reaction. RSC Advances, 2018, 8, 15595-15602.	1.7	9
52	Theoretical Study on a Potential Oxygen Reduction Reaction Electrocatalyst: Single Fe Atoms Supported on Graphite Carbonitride. Langmuir, 2021, 37, 428-436.	1.6	9
53	Radical reaction HCNOÂ+Â3NH: a mechanistic study. Theoretical Chemistry Accounts, 2009, 124, 123-137.	0.5	8
54	Ambipolar charge-transport properties in 4,10-dihalogenated anthanthrone crystals: a theoretical study. Journal of Materials Chemistry C, 2015, 3, 1913-1921.	2.7	8

#	Article	IF	Citations
55	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.	2.7	7
56	Accurate potential surfaces for the ground state of H+C2 reaction. European Physical Journal D, 2017, 71, 1.	0.6	7
57	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.	2.7	7
58	Realizing Efficient Catalytic Performance and High Selectivity for Oxygen Reduction Reaction on a 2D Ni₂SbTe₂ Monolayer. Inorganic Chemistry, 2022, 61, 2284-2291.	1.9	7
59	Theoretical study on reaction mechanism of the CF radical with nitrogen dioxide. Journal of Computational Chemistry, 2001, 22, 1907-1919.	1.5	6
60	Theoretical studies on structures and stabilities of C4H2 + isomers. Chemical Research in Chinese Universities, 2013, 29, 150-153.	1.3	6
61	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.	0.8	6
62	DFT study on the iridium-catalyzed multi-alkylation of alcohol with ammonia. RSC Advances, 2016, 6, 87362-87372.	1.7	6
63	Reaction mechanisms of methanol oxidation by <scp>Fe^{IV}O</scp> biomimetic complex. International Journal of Quantum Chemistry, 2016, 116, 692-701.	1.0	6
64	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.	1.7	6
65	Theoretical Mechanistic Study on the Ionâ˙Molecule Reactions of CCN+/CNC+with H2S. Journal of Physical Chemistry A, 2002, 106, 2949-2962.	1.1	5
66	A Theoretical Study on the Potential Energy Surface of the 3C2 + NO Reaction. Journal of Physical Chemistry A, 2004, 108, 6771-6777.	1.1	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. Structural Chemistry, 2014, 25, 1343-1357.	1.0	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. Structural Chemistry, 2015, 26, 951-959.	1.0	5
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.	1.4	5
70	Unique Electronic Structure in a Porous Gaâ€In Bimetallic Oxide Nanoâ€Photocatalyst with Atomically Thin Pore Walls. Angewandte Chemie, 2016, 128, 11614-11618.	1.6	5
71	Methanol dissociation and oxidation on single Fe atom supported on graphitic carbon nitride. Applied Organometallic Chemistry, 2019, 33, e4930.	1.7	5
72	Theoretical study of substituent effects on electride characteristics and the nonlinear optical properties of Li@calix[4]pyrrole. RSC Advances, 2019, 9, 37919-37925.	1.7	5

#	Article	IF	Citations
73	Molecular dynamics simulations investigate the pathway of substrate entry active site of rhomboid protease. Journal of Biomolecular Structure and Dynamics, 2019, 37, 3445-3455.	2.0	5
74	Global accurate diabatic potential surfaces for the reaction H + Li₂. RSC Advances, 2020, 10, 39226-39240.	1.7	5
75	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.	2.1	5
76	Theoretical study of the hydrogen abstraction by chlorine atoms for CH2BrCl and CHBrCl2. Physical Chemistry Chemical Physics, 2002, 4, 46-50.	1.3	4
77	Atomic radicalâ€"molecule reactions F +Â CH3Câ‰¡CH: mechanistic study. Theoretical Chemistry Accounts, 2007, 117, 417-429.	0.5	4
78	Structure and Stability of Interstellar Molecule C₃S. Chinese Journal of Chemistry, 2002, 20, 1487-1493.	2.6	4
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.	1.0	4
80	Theoretical study of the potential-energy surface of C 2 NP. Theoretical Chemistry Accounts, 2001, 107, 1-7.	0.5	3
81	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.	1.3	3
82	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.	0.5	3
83	A barrier-free molecular radical-molecule reaction: $${^{3}C_{2} (a^{3}Pi) {+} O_{2} (X^{3}) Tj ETQq1 1 0.784314 rgBT /Overlock 1	0.5	3
84	Theoretical study on the structures, isomerization and stability of SiC4 isomers. Theoretical Chemistry Accounts, 2010, 126, 15-25.	0.5	3
85	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
86	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.	1.3	3
87	Reactive scattering for Dâˆ' + D2 (v = 0â€"1, j = 0â€"8): quantum and classical trajectory investigation. European Physical Journal D, 2014, 68, 1.	0.6	3
88	Structures and nonlinear optical properties of lithium-adsorbed polycyclic Ï€-conjugated pentacene systems. Chemical Research in Chinese Universities, 2015, 31, 261-269.	1.3	3
89	Reactive scattering for Hâˆ'â€‰+â€‰HD and Dâˆ'â€‰+â€‰HD: classical trajectory investigation. European Physical Journal D, 2015, 69, 1.	0.6	3
90	Investigations of Takeout proteinsâ€™ ligand binding and release mechanism using molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1464-1473.	2.0	3

#	Article	IF	Citations
91	Dissociation and oxidation mechanism of methanol on Al12N12 cage: a DFT study. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	3
92	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.	0.5	3
93	Theoretical study of a novel organic electride with large nonlinear optical responses. International Journal of Quantum Chemistry, 2020, 120, e26235.	1.0	3
94	Heteroatom-doped fullerene C70 as non-metal electrocatalysts for oxygen reduction and oxygen evolution from computational study. Diamond and Related Materials, 2022, 124, 108954.	1.8	3
95	Molecular dynamics simulation of polystyrene-block-poly(methyl methacrylate). Macromolecular Theory and Simulations, 1998, 7, 619-622.	0.6	2
96	Tree-gel and loop-gel conversions in nonlinear polymerization. Science in China Series B: Chemistry, 1998, 41, 122-134.	0.8	2
97	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
98	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.	1.2	2
99	Structure and Stability of Isomers of the Promising Interstellar Molecule PC3O. Theoretical Chemistry Accounts, 2006, 115, 410-426.	0.5	2
100	Theoretical study of the Si2NO potential energy surface. International Journal of Quantum Chemistry, 2007, 107, 1181-1193.	1.0	2
101	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.	0.5	2
102	A barrierâ€free atomic radicalâ€molecule reaction: N (²D) NO₂ (²A₁) mechanistic study. International Journal of Quantum Chemistry, 2008, 108, 1309-1315.	1.0	2
103	The adsorption of poly (vinyl alcohol) on the hydroxylated Î²-cristobalite. Molecular Simulation, 2008, 34, 611-618.	0.9	2
104	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
105	Theoretical study on the mechanism of C2Cl3Â+ÂNO2 reaction. Theoretical Chemistry Accounts, 2009, 123, 431-441.	0.5	2
106	Structures and Stability of HNS2 Isomers. Chinese Journal of Chemistry, 2010, 20, 760-765.	2.6	2
107	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.	0.1	2
108	The mechanism investigation of the imidazolidinone catalyzed fiveâ€membered ring synthesis reaction. Journal of Physical Organic Chemistry, 2013, 26, 232-239.	0.9	2

#	Article	IF	Citations
109	Theoretical investigation on the reaction of HS+ with CH3NH2. Chemical Papers, 2014, 68, .	1.0	2
110	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.	0.8	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.	2.0	2
112	Exploring the Mechanism of the Palladium-Catalyzed 3-Butene-2-ol Amination Reaction: A DFT Study. Frontiers in Chemistry, 2020, 8, 48.	1.8	2
113	Catalytic activity of Ruâ€N₄ doped vacancy fullerenes (Ruâ€N₄â€C₅₄) Tj ETQq1 1 0.784314 rgB theory investigation. Applied Organometallic Chemistry, 2022, 36, .	1.7	2
114	Generation of singlet oxygen catalyzed by the room-temperature-stable anthraquinone anion radical. Physical Chemistry Chemical Physics, 2022, 24, 14165-14171.	1.3	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.	0.8	1
117	Theoretical study on the potential energy surface of NC3P isomers. Theoretical Chemistry Accounts, 2007, 118, 739-754.	0.5	1
118	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
119	Theoretical study on the ionâ€“molecule reaction of HCN+ with NH3. Theoretical Chemistry Accounts, 2009, 124, 409-420.	0.5	1
120	Direct dynamic study on the hydrogen abstraction reaction of H₂CO with NCO. International Journal of Chemical Kinetics, 2009, 41, 394-400.	1.0	1
121	Reactive scattering for H+ + H2: non-Born-Oppenheimer classical investigation. European Physical Journal D, 2013, 67, 1.	0.6	1
122	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.	7.8	1
123	Theoretical investigation on the mechanism of FeCl3-catalysed cross-coupling reaction of alcohols with alkenes. Molecular Physics, 2014, 112, 2107-2113.	0.8	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.	0.9	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.	2.0	1
126	Conformational transitions of uracil transporter UraA from Escherichia coli: a molecular simulation study. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3398-3410.	2.0	1

#	Article	IF	Citations
127			