Hong-Xing Zhang

List of Publications by Year
in descending order

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160 papers	3,124 citations	201674 27 h-index	206112 48 g-index
162 all docs	162 docs citations	162 times ranked	4481 citing authors

#	Article	IF	Citations
1	Atomic Modulation of FeCoâ€“Nitrogenâ€“Carbon Bifunctional Oxygen Electrodes for Rechargeable and Flexible Allâ€Solidâ€State Zincâ€“Air Battery. Advanced Energy Materials, 2017, 7, 1602420.	19.5	692
2	Hole Trapping by Iodine Interstitial Defects Decreases Free Carrier Losses in Perovskite Solar Cells: A Time-Domain Ab Initio Study. ACS Energy Letters, 2017, 2, 1270-1278.	17.4	151
3	Theoretical Studies of the Absorption and Emission Properties of the Fluorene-Based Conjugated Polymers. Macromolecules, 2004, 37, 3451-3458.	4.8	90
4	Controlling Metallophilic Interactions in Chiral Gold(I) Double Salts towards Excitation Wavelengthâ€Tunable Circularly Polarized Luminescence. Angewandte Chemie - International Edition, 2020, 59, 6915-6922.	13.8	71
5	What Makes Hydroxamate a Promising Anchoring Group in Dye-Sensitized Solar Cells? Insights from Theoretical Investigation. Journal of Physical Chemistry Letters, 2014, 5, 3992-3999.	4.6	61
6	Enamineâ€“Metal Lewis Acid Bifunctional Catalysis: Application to Direct Asymmetric Aldol Reaction of Ketones. European Journal of Organic Chemistry, 2009, 2009, 4581-4585.	2.4	53
7	An External Electric Field Manipulated Second-Order Nonlinear Optical Switch of an Electride Molecule: A Long-Range Electron Transfer Forms a Lone Excess Electron Pair and Quenches Singlet Diradical. Journal of Physical Chemistry C, 2016, 120, 13656-13666.	3.1	50
8	Design of Dâ€“Aâ€“Ï€â€“A organic dyes with different acceptor and auxiliary acceptor for highly efficient dye-sensitized solar cells: a computational study. RSC Advances, 2014, 4, 50338-50350.	3.6	43
9	A Theoretical Investigation of Substituent Effects on the Absorption and Emission Properties of a Series of Terpyridylplatinum(II) Acetylide Complexes. European Journal of Inorganic Chemistry, 2005, 2005, 1856-1866.	2.0	40
10	Investigation of Properties of Mg_n Clusters and Their Hydrogen Storage Mechanism: A Study Based on DFT and a Global Minimum Optimization Method. Journal of Physical Chemistry A, 2015, 119, 3636-3643.	2.5	40
11	Comprehensive Investigation into Luminescent Properties of Ir(III) Complexes: An Integrated Computational Study of Radiative and Nonradiative Decay Processes. Inorganic Chemistry, 2018, 57, 6561-6570.	4.0	40
12	Ab initio Study on Luminescence and Aurophilicity of a Dinuclear [(AuPH3)2(i-mnt)] Complex (i-mnt =) Tj ETQq0 0 0 rgBT /Overlock 10 T	2.6	37
13	Molecular Dynamic Investigations of the Mutational Effects on Structural Characteristics and Tunnel Geometry in CYP17A1. Journal of Chemical Information and Modeling, 2013, 53, 3308-3317.	5.4	37
14	Theoretical study and design of highly efficient platinum(<scp>ii</scp>) complexes bearing tetradentate ligands for OLED. RSC Advances, 2016, 6, 11648-11656.	3.6	37
15	Efficient Blue-Emitting Ir(III) Complexes with Phosphine Carbanion-Based Ancillary Ligand: A DFT Study. Journal of Physical Chemistry A, 2011, 115, 11689-11695.	2.5	35
16	DFT and TD-DFT study on the electronic structures and phosphorescent properties of 6-phenyl-2,2â€²-bipyridine tridentate iridium(iii) complexes and their isomer. Dalton Transactions, 2012, 41, 8441.	3.3	34
17	Anionic ancillary ligands in cyclometalated Ru(<scp>ii</scp>) complex sensitizers improve photovoltaic efficiency of dye-sensitized solar cells: insights from theoretical investigations. Journal of Materials Chemistry A, 2017, 5, 15567-15577.	10.3	33
18	Promising pyridinium ylide based anchors towards high-efficiency dyes for dye-sensitized solar cells applications: Insights from theoretical investigations. Electrochimica Acta, 2018, 283, 1798-1805.	5.2	33

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19	The influence of an inner electric field on the performance of three types of Zn-porphyrin sensitizers in dye sensitized solar cells: a theoretical study. Journal of Materials Chemistry C, 2016, 4, 10130-10145.	5.5	31
20	Investigation of the adsorption properties of gemcitabine anticancer drug with metal-doped boron nitride fullerenes as a drug-delivery carrier: a DFT study. RSC Advances, 2022, 12, 2873-2887.	3.6	31
21	Theoretical research on the effect of regulated Ï€-conjugation on the photophysical properties of Ir(<scp>iii</scp>) complexes. Physical Chemistry Chemical Physics, 2015, 17, 10014-10021.	2.8	30
22	Theoretical studies on the spectroscopic properties of porphyrin derivatives for dye-sensitized solar cell application. RSC Advances, 2015, 5, 33653-33665.	3.6	30
23	Disentangling the role of oxygen vacancies on the surface of Fe₃O₄ and Î³-Fe₂O₃. Inorganic Chemistry Frontiers, 2019, 6, 2660-2666.	6.0	30
24	Electronic structures and optical properties of neutral substituted fluorene-based cyclometalated platinum(II)â€“acetylide complexes: A DFT exploration. Journal of Organometallic Chemistry, 2009, 694, 1848-1860.	1.8	29
25	A theoretical analysis of the phosphorescence efficiencies of Cu(<scp>i</scp>) complexes. Dalton Transactions, 2014, 43, 11252-11259.	3.3	29
26	The influence of a dyeâ€“TiO₂ interface on DSSC performance: a theoretical exploration with a ruthenium dye. RSC Advances, 2016, 6, 81976-81982.	3.6	28
27	Novel Carbon Nanotubes Rolled from 6,6,12-Graphyne: Double Dirac Points in 1D Material. Journal of Physical Chemistry C, 2017, 121, 14835-14844.	3.1	28
28	A highly selective fluorescent probe for cyanide ion and its detection mechanism from theoretical calculations. Talanta, 2018, 185, 1-6.	5.5	28
29	Rational design of metal-free organic D-Ï€-A dyes in dye-sensitized solar cells: Insight from density functional theory (DFT) and time-dependent DFT (TD-DFT) investigations. Organic Electronics, 2018, 59, 131-139.	2.6	28
30	Molecular Dynamics Simulations Suggest Ligandâ€™s Binding to Nicotinamidase/Pyrazinamidase. PLoS ONE, 2012, 7, e39546.	2.5	28
31	Theoretical investigation of the adsorption, IR, and electron injection of hydroxamate anchor at the TiO₂ anatase (1 0 1) surface. RSC Advances, 2014, 4, 19690-19693.	3.6	26
32	How does graphene enhance the photoelectric conversion efficiency of dye sensitized solar cells? An insight from a theoretical perspective. Journal of Materials Chemistry A, 2019, 7, 2730-2740.	10.3	26
33	A novel T-C₃N and seawater desalination. Nanoscale, 2020, 12, 5055-5066.	5.6	26
34	Theoretical investigation on the effect of ancillary ligand modification for highly efficient phosphorescent platinum(<scp>ii</scp>) complex design. RSC Advances, 2017, 7, 17368-17376.	3.6	25
35	DFT/TD-DFT calculations on the sensing mechanism of a dual response near-infrared fluorescent chemosensor for superoxide anion and hydrogen polysulfides: photoinduced electron transfer. RSC Advances, 2016, 6, 104735-104741.	3.6	23
36	Lighting Silver(I) Complexes for Solution-Processed Organic Light-Emitting Diodes and Biological Applications via Thermally Activated Delayed Fluorescence. Inorganic Chemistry, 2020, 59, 12122-12131.	4.0	23

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37	Theoretical studies of the spectroscopic properties of blue emitting iridium complexes. Theoretical Chemistry Accounts, 2008, 121, 155-164.	1.4	22
38	A theoretical study on the thermal cisâ€“trans isomerization of azoheteroarene photoswitches. New Journal of Chemistry, 2017, 41, 1659-1669.	2.8	22
39	The effect of Dâ€“[D_eâ€“Ï€â€“A]_n (n = 1, 2, 3) type dyes on the overall performance of DSSCs: a theoretical investigation. Journal of Materials Chemistry C, 2017, 5, 7510-7520.	5.5	22
40	Controllable molecular aggregation and fluorescence properties of 1,3,4-oxadiazole derivatives. Journal of Materials Chemistry C, 2015, 3, 11681-11688.	5.5	21
41	Control of Charge Carrier Dynamics in Plasmonic Au Films by TiO_x Substrate Stoichiometry. Journal of Physical Chemistry Letters, 2020, 11, 1419-1427.	4.6	21
42	DFT/TDDFT investigation of the electronic structures and optoelectronic properties of phosphorescent iridium (III) complexes with non-conjugated cyclometalated carbene ligands. Molecular Physics, 2011, 109, 1657-1675.	1.7	20
43	Structural features and dynamic investigations of the membrane-bound cytochrome P450 17A1. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 2013-2021.	2.6	20
44	How the substituents in corannulene and sumanene derivatives alter their molecular assemblings and charge transport properties?-A theoretical study with a dimer model. Journal of Computational Chemistry, 2016, 37, 813-824.	3.3	20
45	The effect of the embedded o-carborane ligand on the photophysical properties of a cyclometalated Pt(<scp>ii</scp>) complex: a theoretical investigation. Inorganic Chemistry Frontiers, 2018, 5, 1016-1025.	6.0	20
46	Performance Regulation of Thieno[3,2-b]benzothiophene Ï€-Spacer-Based D-Ï€-A Organic Dyes for Dye-Sensitized Solar Cell Applications: Insights From Computational Study. Frontiers in Chemistry, 2018, 6, 676.	3.6	20
47	Revealing the binding and drug resistance mechanism of amprenavir, indinavir, ritonavir, and nelfinavir complexed with HIV-1 protease due to double mutations G48T/L89M by molecular dynamics simulations and free energy analyses. Physical Chemistry Chemical Physics, 2020, 22, 4464-4480.	2.8	20
48	Investigation of ligand selectivity in CYP3A7 by molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2015, 33, 2360-2367.	3.5	19
49	Toward highly fluorescence and ultralow-threshold amplified spontaneous emission in ordered solid state from twin-tapered bi-1,3,4-oxadiazole derivatives. Journal of Materials Chemistry, 2012, 22, 3875.	6.7	18
50	Molecular-Level Insight of Cu(I) Complexes with the 7,8-Bis(diphenylphosphino)-7,8-dicarba-nido-undecaborate Ligand as a Thermally Activated Delayed Fluorescence Emitter: Luminescent Mechanism and Design Strategy. Inorganic Chemistry, 2020, 59, 12039-12053.	4.0	18
51	Theoretical Studies of the Electronic Structure and Spectroscopic Properties of [Ru(Htcterpy)(NCS)3]3â€“. European Journal of Inorganic Chemistry, 2007, 2007, 2171-2180.	2.0	17
52	Detoxification of 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP) by cytochrome P450 enzymes: A theoretical investigation. Journal of Inorganic Biochemistry, 2016, 154, 21-28.	3.5	17
53	A Computational Way To Achieve More Effective Candidates for Photodynamic Therapy. Journal of Chemical Information and Modeling, 2017, 57, 1089-1100.	5.4	17
54	A complete evaluation from theoretical aspect on the phosphorescent efficiency improvement through ancillary ligands modifications of a blue Ir(III) complex. Organic Electronics, 2018, 59, 293-300.	2.6	17

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55	MD Simulation Investigation on the Binding Process of Smoke-Derived Germination Stimulants to Its Receptor. Journal of Chemical Information and Modeling, 2019, 59, 1554-1562.	5.4	17
56	Exploring the interactional details between aldose reductase (AKR1B1) and 3-Mercapto-5H-1,2,4-triazino[5,6-b]indole-5-acetic acid through molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1724-1735.	3.5	17
57	Arranging strategies for A-site cations: impact on the stability and carrier migration of hybrid perovskite materials. Inorganic Chemistry Frontiers, 2020, 7, 1741-1749.	6.0	17
58	Molecular design of organic dyes with diketopyrrolopyrrole for dyeâ€sensitized solar cell: A theoretical approach. International Journal of Quantum Chemistry, 2014, 114, 560-567.	2.0	16
59	Theoretical studies of heteroatom-doping in TiO₂ to enhance the electron injection in dye-sensitized solar cells. RSC Advances, 2015, 5, 79868-79873.	3.6	16
60	Computational Studies on the Materials Combining Graphene Quantum Dots and Pt Complexes with Adjustable Luminescence Characteristics. Inorganic Chemistry, 2021, 60, 1480-1490.	4.0	16
61	Density functional study on the effect of substituent group for the monomer of donorâ€acceptor copolymer. Journal of Polymer Science, Part B: Polymer Physics, 2010, 48, 2099-2107.	2.1	15
62	Direct evidence for the effect of lateral hydrogen bonding on the smectic phase. Liquid Crystals, 2011, 38, 767-774.	2.2	15
63	Theoretical study on the excited state decay properties of iron(<scp>ii</scp>) polypyridine complexes substituted by bromine and chlorine. RSC Advances, 2019, 9, 31621-31627.	3.6	15
64	The impact of molecular stacking interactions on the electronic structure and charge transport properties in distyrylbenzene (DSB-) based Dâ€“A complexes: a theoretical study. RSC Advances, 2015, 5, 47681-47691.	3.6	14
65	Two cationic [(Cu_xI_y)^{xâ^'y}]_n motif based coordination polymers and their photocatalytic properties. RSC Advances, 2016, 6, 71206-71213.	3.6	14
66	Intrinsic quantum efficiency enhancement in well-known Ir(iii) complexes by virtue of a simple and controllable deuteriation strategy. Materials Chemistry Frontiers, 2018, 2, 1215-1224.	5.9	14
67	Theoretical Studies on Metalâ€“Metal Interaction and Intrinsic1,3[Ïƒ*(d)Ïƒ(s/p)] Excited States of Dinuclear d10 Complexes with Bridging Phosphane Ligands. European Journal of Inorganic Chemistry, 2006, 2006, 1050-1059.	2.0	13
68	Electronic Structures and Spectroscopic Properties of [Pt(CNMe)2(CN)2]n (n = 1â€“4): A Theoretical Exploration of Promising Phosphorescent Materials. European Journal of Inorganic Chemistry, 2007, 2007, 2181-2188.	2.0	13
69	Strategies on Cyclometalating Ligand Substitution of Several Ir(III) Complexes: Theoretical Investigation of Different Molecular Behaviors. Organometallics, 2018, 37, 2491-2499.	2.3	13
70	Theoretical study on organic dyes with tunable Ï€-spacers for dye-sensitized solar cells: Inspired by the organic polymer photovoltaics. Chemical Physics Letters, 2019, 719, 39-44.	2.6	13
71	How Does (E)-2-(Acetamidomethylene)succinate Bind to Its Hydrolase? From the Binding Process to the Final Result. PLoS ONE, 2013, 8, e53811.	2.5	12
72	Theoretical investigation on a series of novel S,S-dioxide diarylethenes with abnormal photochromic properties and design of new dyads. New Journal of Chemistry, 2015, 39, 1634-1642.	2.8	12

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73	Iron oxides with a reverse spinel structure: impact of active sites on molecule adsorption. Inorganic Chemistry Frontiers, 2019, 6, 2810-2816.	6.0	12
74	Dihydrogen bond in C2H4â^'nClnâ€‰Â·Â·Â·â€‰NaH (nâ€‰=â€‰0,â€‰1,â€‰2,â€‰3) complexes: ab initio, AIM and NBO studies. Physics, 2011, 109, 645-653.	1.7	11
75	Theoretical Investigation on Excited-State Cyclization Reactions of Platinum-Sensitized Dithienylethene Complexes. Journal of Physical Chemistry A, 2015, 119, 2819-2828.	2.5	11
76	Exploring the interaction between human focal adhesion kinase and inhibitors: a molecular dynamic simulation and free energy calculations. Journal of Biomolecular Structure and Dynamics, 2016, 34, 2351-2366.	3.5	11
77	The phosphorescence properties of a series of diarylethene-containing platinum complexes: the effect of ligand photoisomerization. Organic Chemistry Frontiers, 2017, 4, 2191-2201.	4.5	11
78	Conformational Transition of Key Structural Features Involved in Activation of ALK Induced by Two Neuroblastoma Mutations and ATP Binding: Insight from Accelerated Molecular Dynamics Simulations. ACS Chemical Neuroscience, 2018, 9, 1783-1792.	3.5	11
79	In Silico Study of Membrane Lipid Composition Regulating Conformation and Hydration of Influenza Virus B M2 Channel. Journal of Chemical Information and Modeling, 2020, 60, 3603-3615.	5.4	11
80	Drug Design Benefits from Molecular Dynamics: Some Examples. Current Computer-Aided Drug Design, 2013, 9, 532-546.	1.2	11
81	Theoretical Studies on [Ru(bpy)₂(NN)]²⁺ [NN = Hydrazone and Azine]: Groundâ€• and Excitedâ€Šstate Geometries, Electronic Structures, Absorptions, and Phosphorescence Mechanisms. European Journal of Inorganic Chemistry, 2008, 2008, 1268-1276.	2.0	10
82	A CASSCF/CASPT2 study on the low-lying excited states of HSiCN, HSiNC and their ions. Theoretical Chemistry Accounts, 2009, 124, 85-93.	1.4	10
83	The induced current strengths and aromatic pathways of heteroporphyrins and their antiaromatic derivatives. International Journal of Quantum Chemistry, 2015, 115, 983-988.	2.0	10
84	Geometries and stabilities of Ag n v (vÂ=ÂÂ±1, 0; nÂ=Â21â€“29) clusters. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	9
85	Theoretical studies of the reaction of hydroxyl radical with cyclopentane (C5H10). Molecular Physics, 2014, 112, 963-971.	1.7	9
86	Regulating ancillary ligands of Ru(<scp>ii</scp>) complexes with square-planar quadridentate ligands for more efficient sensitizers in dye-sensitized solar cells: insights from theoretical investigations. Physical Chemistry Chemical Physics, 2016, 18, 29591-29599.	2.8	9
87	Theoretical study on the neutral and ionic Cu(I) phosphorescent complexes with 2-(2â€²-quinolyl)benzimidazole and phosphine mixed ligand. Organic Electronics, 2016, 31, 111-119.	2.6	9
88	Study on the spectral complementary composite dye molecules designed for high performance dye-sensitized solar cells: A theoretical investigation. Computational and Theoretical Chemistry, 2019, 1154, 44-49.	2.5	9
89	STABILITIES AND FRAGMENTATION BEHAVIORS OF Agn CLUSTERS (n = 2â€“34). Journal of Theoretical and Computational Chemistry, 2012, 11, 953-964.	1.8	8
90	Bisactinyl halogenated complexes: relativistic density functional theory calculation and experimental synthesis. RSC Advances, 2013, 3, 1572-1582.	3.6	8

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91	Theoretical study on the electronic structures and properties of diindolocarbazole isomers. Journal of Physical Organic Chemistry, 2014, 27, 973-980.	1.9	8
92	Theoretical study of the cisâ€“trans isomerization mechanism of a pendant metal-bound azobenzene. RSC Advances, 2016, 6, 79879-79889.	3.6	8
93	Probing the interaction mechanism of small molecule inhibitors with matriptase based on molecular dynamics simulation and free energy calculations. Journal of Biomolecular Structure and Dynamics, 2017, 35, 755-764.	3.5	8
94	Theoretical Study on the Photoinduced Electron Transfer Mechanisms of Different Peroxynitrite Probes. Journal of Physical Chemistry A, 2018, 122, 217-223.	2.5	8
95	Interaction Mechanism of the Germination Stimulants Karrikins and Their Receptor ShKAI2iB. Journal of Physical Chemistry B, 2020, 124, 9812-9819.	2.6	8
96	Mutation and low pH effect on the stability as well as unfolding kinetics of transthyretin dimer. Biophysical Chemistry, 2014, 189, 8-15.	2.8	7
97	Theoretical study on molecular packing and electronic structure of bi-1,3,4-oxadiazole derivatives. RSC Advances, 2014, 4, 51942-51949.	3.6	7
98	Enhancing Electron Injection in Dyeâ€Sensitized Solar Cells by Adopting W⁶⁺â€Doped TiO₂ Nanowires: A Theoretical Study. European Journal of Inorganic Chemistry, 2015, 2015, 5563-5570.	2.0	7
99	Exploring the sensitization properties of thienyl-functionalized tripyrrole Ru(II) complexes on TiO2 (101) surface: a theoretical study. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	7
100	Exploring the structure characteristics and major channels of cytochrome P450 2A6, 2A13, and 2E1 with pilocarpine. Biopolymers, 2018, 109, e23108.	2.4	7
101	Molecular Dynamics Simulation Investigation of the Binding and Interaction of the EphA6â€“Odin Protein Complex. Journal of Physical Chemistry B, 2022, 126, 4914-4924.	2.6	7
102	Computational studies on the spectroscopic properties of the 2â€pyridylpyrazolateâ€based platinum(II) complexes with modified pyrazolate fragment. International Journal of Quantum Chemistry, 2009, 109, 308-319.	2.0	6
103	Homology modelling and molecular dynamics study of human fatty acid amide hydrolase. Molecular Simulation, 2009, 35, 1201-1208.	2.0	6
104	CASPT2 and CASSCF studies on the low-lying electronic states of the HCCO radical and its anion. Theoretical Chemistry Accounts, 2010, 125, 65-73.	1.4	6
105	Low-lying electronic states of HNCS and its ions: a CASSCF/CASPT2 study. Theoretical Chemistry Accounts, 2011, 128, 215-222.	1.4	6
106	Quantum chemical modeling of 1,1â€proton transfer reaction catalyzed by a cofactorâ€independent Î±â€methylacylâ€CoA racemase. International Journal of Quantum Chemistry, 2012, 112, 619-624.	2.0	6
107	Molecular dynamics investigations of BioH protein substrate specificity for biotin synthesis. Journal of Biomolecular Structure and Dynamics, 2016, 34, 1052-1060.	3.5	6
108	Exploring the inhibition mechanism on HIFâ€2 by inhibitor PT2399 and 0X3 using molecular dynamics simulations. Journal of Molecular Recognition, 2018, 31, e2730.	2.1	6

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109	Defect Interaction and Deformation in Graphene. Journal of Physical Chemistry C, 2020, 124, 2370-2378.	3.1	6
110	Theoretical studies on the electronic structures and spectroscopic properties for a series of Osmium(II)-2,2â€²,6â€²,2â€²â€²-terpyridine complexes. Theoretical Chemistry Accounts, 2008, 121, 123-134.	1.4	5
111	Theoretical investigation on the spectroscopic properties of cyclometallated iridium (III) complexes and the deprotonation influence on them in solution. International Journal of Quantum Chemistry, 2011, 111, 4080-4090.	2.0	5
112	A CASSCF/CASPT2 study on the lowâ€lying electronic states of the CH₃SS and its cation. International Journal of Quantum Chemistry, 2012, 112, 1537-1546.	2.0	5
113	Theoretical studies of the structural, electronic and optical properties of carbazoleâ€based compounds. Journal of Physical Organic Chemistry, 2012, 25, 334-342.	1.9	5
114	Theoretical studies on structural and spectroscopic properties of photoelectrochemical cell ruthenium sensitizers, derivatives of AR20. International Journal of Quantum Chemistry, 2013, 113, 891-901.	2.0	5
115	Molecular dynamics (MD) simulations and binding free energy calculation studies between inhibitors and type II dehydroquinase (DHQ2). Molecular Simulation, 2013, 39, 137-144.	2.0	5
116	Exploring the mechanism how AF9 recognizes and binds H3K9ac by molecular dynamics simulations and free energy calculations. Biopolymers, 2016, 105, 779-786.	2.4	5
117	Effect of External Electric Field on Substrate Transport of a Secondary Active Transporter. Journal of Chemical Information and Modeling, 2016, 56, 1539-1546.	5.4	5
118	Theoretical studies on electronic structures and spectroscopic properties of a series of novel Î²-diketonate Os(II) complexes. Theoretical Chemistry Accounts, 2009, 122, 31-42.	1.4	4
119	HOMOLOGY MODELING AND SUBSTRATE BINDING STUDY OF HUMAN KYNURENINE AMINOTRANSFERASE III. Journal of Theoretical and Computational Chemistry, 2012, 11, 855-870.	1.8	4
120	Computational study on zinc porphyrin analogs for use in dye-sensitized solar cells. Journal of Porphyrins and Phthalocyanines, 2014, 18, 406-415.	0.8	4
121	Theoretical investigation on remote-control photocycloreversion of dithienylethene driven by azobenzene chromophores. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 137, 987-994.	3.9	4
122	Molecular dynamics investigation of stereoselective inhibition mechanism of HIFâ€2Î±/ARNT heterodimer. Journal of Molecular Recognition, 2018, 31, e2675.	2.1	4
123	Insight on mutationâ€induced resistance to anaplastic lymphoma kinase inhibitor ceritinib from molecular dynamics simulations. Biopolymers, 2019, 110, e23257.	2.4	4
124	Ab initio and DFT study of the electronic structures and spectroscopic properties of pyrene ligands and their cyclometalated complexes. International Journal of Quantum Chemistry, 2011, 111, 2258-2267.	2.0	3
125	A comparative analysis of binding sites between human PKD1 and PKC1 based on homology modelling, molecular dynamics simulation and docking studies. Molecular Simulation, 2012, 38, 309-314.	2.0	3
126	Molecular dynamic studies on Langmuir monolayers of stearic acid. Chemical Research in Chinese Universities, 2013, 29, 545-550.	2.6	3

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127	Theoretical analysis on magnetic properties of conjugated organic molecules containing borepin. Chemical Research in Chinese Universities, 2013, 29, 962-968.	2.6	3
128	Theoretical analysis of electrochromism under redox of bis(3-thienyl)/(2-thienyl)hexafluorocyclopentene: effects of charged and substituted systems. Physical Chemistry Chemical Physics, 2017, 19, 9281-9291.	2.8	3
129	Zincâ€Air Batteries: Atomic Modulation of FeCoâ€“Nitrogenâ€“Carbon Bifunctional Oxygen Electrodes for Rechargeable and Flexible Allâ€Solidâ€State Zincâ€“Air Battery (Adv. Energy Mater. 13/2017). Advanced Energy Materials, 2017, 7, .	19.5	3
130	A density functional theory investigation of the stability, aromaticity, and photophysical behavior for the highly conjugated macrocycles containing 4 pyrroles. Journal of Physical Organic Chemistry, 2017, 30, e3617.	1.9	3
131	Molecular dynamics simulations study of influence of Tyr422Ala mutation on transcriptional enhancer activation domain 4 (TEAD4) and transcription co-activators complexes. Journal of Theoretical Biology, 2019, 472, 27-35.	1.7	3
132	Probing the effect of substituent groups in Ir(III) bis-tridentate complexes during deep-blue phosphorescent illuminating. Organic Electronics, 2020, 84, 105803.	2.6	3
133	Theoretical Design of cisâ€Bis(imido)uranium Iodides â€“ Electronic Structures and Spectroscopic Properties. European Journal of Inorganic Chemistry, 2014, 2014, 5168-5176.	2.0	2
134	Molecular basis of the recognition of FMN by a HAD phosphatase TON_0338. Journal of Molecular Graphics and Modelling, 2016, 69, 17-25.	2.4	2
135	Why HSâ^' and CNâ^' can be detected by different chemosensors with similar structures: a quantum mechanics and molecular dynamics study. RSC Advances, 2016, 6, 63548-63558.	3.6	2
136	Studying the recognition mechanism of TcaR and ssDNA using molecular dynamic simulations. Journal of Molecular Graphics and Modelling, 2018, 80, 67-75.	2.4	2
137	Recognition mechanism of Wilmsâ€™ tumour suppressor protein and DNA triplets: insights from molecular dynamics simulation and free energy analysis. Journal of Biomolecular Structure and Dynamics, 2019, 37, 562-575.	3.5	2
138	Mechanism of A pH-induced Peptide Inserting into a POPC Bilayer: A Molecular Dynamic Study. Current Pharmaceutical Biotechnology, 2014, 15, 814-822.	1.6	2
139	Comparative study on the photophysical properties between carbeneâ€based Fe (II) and Ru (II) complexes. Applied Organometallic Chemistry, 2020, 34, .	3.5	2
140	Accurate Analysis of Anisotropic Carrier Mobility and Structureâ€“property Relationships in Organic BOXD Crystalline Materials. Frontiers in Chemistry, 2021, 9, 775747.	3.6	2
141	Molecular Basis of the Recognition of Cholesterol by Cytochrome P450 46A1 along the Major Access Tunnel. ACS Chemical Neuroscience, 2022, , .	3.5	2
142	Two topological approaches to resonance energy and the relation between them. Chinese Journal of Chemistry, 1989, 7, 324-332.	0.0	1
143	A quantum mechanics study on the reaction mechanism of chalcone formation from p-coumaroyl-CoA and malonyl-CoA catalyzed by chalcone synthase. Theoretical Chemistry Accounts, 2009, 122, 157-166.	1.4	1
144	Electronic structures and spectroscopic properties of promising highly efficient red phosphorescent Os(II)(LR)2(PH3)2 complexes: a theoretical exploration. Theoretical Chemistry Accounts, 2010, 127, 467-474.	1.4	1

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