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	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
2	Refine the evaluation of photophysical properties of organometallic chromophores under confined molecular crystal conditions. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 275, 121168.	3.9	1
3	Molecular Basis of the Recognition of Cholesterol by Cytochrome P450 46A1 along the Major Access Tunnel. ACS Chemical Neuroscience, 2022, , .	3.5	2
4	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
5	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
6	Computational insight into newly anomalous delayed fluorescence emitters based on D-A-A structures. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 250, 119392.	3.9	0
7	Predicting a Kind of Unusual Multiple-States Dimerization-Modes Transformation in Protein PD-L1 System by Computational Investigation and a Generalized Rate Theory. Frontiers in Chemistry, 2021, 9, 783444.	3.6	1
8	Accurate Analysis of Anisotropic Carrier Mobility and Structureâ€“property Relationships in Organic BOXD Crystalline Materials. Frontiers in Chemistry, 2021, 9, 775747.	3.6	2
9	A DFT study on the mechanism of palladium-catalysed tandem reaction of ortho-electron-deficient alkynyl-substituted aryl aldehydes with indoles. Molecular Physics, 2020, 118, e1576933.	1.7	1
10	Defect Interaction and Deformation in Graphene. Journal of Physical Chemistry C, 2020, 124, 2370-2378.	3.1	6
11	Interesting spin state properties of iron(II) polypyridine complex substituted by fluorine: A theoretical study. Organic Electronics, 2020, 85, 105884.	2.6	1
12	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
13	Interaction Mechanism of the Germination Stimulants Karrikins and Their Receptor ShKAI2iB. Journal of Physical Chemistry B, 2020, 124, 9812-9819.	2.6	8
14	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
15	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
16	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
17	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
18	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

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19	A novel T-C₃N and seawater desalination. Nanoscale, 2020, 12, 5055-5066.	5.6	26
20	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
21	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
22	Comparative study on the photophysical properties between carbeneâ€based Fe (II) and Ru (II) complexes. Applied Organometallic Chemistry, 2020, 34, .	3.5	2
23	Iron oxides with a reverse spinel structure: impact of active sites on molecule adsorption. Inorganic Chemistry Frontiers, 2019, 6, 2810-2816.	6.0	12
24	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
25	Disentangling the role of oxygen vacancies on the surface of Fe₃O₄ and Î³-Fe₂O₃. Inorganic Chemistry Frontiers, 2019, 6, 2660-2666.	6.0	30
26	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
27	Insight on mutationâ€induced resistance to anaplastic lymphoma kinase inhibitor ceritinib from molecular dynamics simulations. Biopolymers, 2019, 110, e23257.	2.4	4
28	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
29	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
30	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
31	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
32	Investigating detailed mechanism of hydrogen molecules adsorbing on singleâ€wall carbon nanotubes using fitted force field parameters containing carbonâ€“carbon interactions. Journal of Computational Chemistry, 2019, 40, 1073-1083.	3.3	0
33	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
34	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
35	Exploring the structure characteristics and major channels of cytochrome P450 2A6, 2A13, and 2E1 with pilocarpine. Biopolymers, 2018, 109, e23108.	2.4	7
36	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

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37	A highly selective fluorescent probe for cyanide ion and its detection mechanism from theoretical calculations. Talanta, 2018, 185, 1-6.	5.5	28
38	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
39	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
40	Molecular dynamics investigation of stereoselective inhibition mechanism of HIFâ€2Î±/ARNT heterodimer. Journal of Molecular Recognition, 2018, 31, e2675.	2.1	4
41	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
42	Theoretical Study on the Photoinduced Electron Transfer Mechanisms of Different Peroxynitrite Probes. Journal of Physical Chemistry A, 2018, 122, 217-223.	2.5	8
43	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
44	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
45	The influence of residue in the position of 116 on the inhibitory potency of TH588 for MTH1. Journal of Molecular Graphics and Modelling, 2018, 85, 75-83.	2.4	0
46	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
47	Strategies on Cyclometalating Ligand Substitution of Several Ir(III) Complexes: Theoretical Investigation of Different Molecular Behaviors. Organometallics, 2018, 37, 2491-2499.	2.3	13
48	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
49	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
50	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
51	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
52	A theoretical study on the thermal cisâ€“trans isomerization of azoheteroarene photoswitches. New Journal of Chemistry, 2017, 41, 1659-1669.	2.8	22
53	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
54	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

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55	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
56	A Computational Way To Achieve More Effective Candidates for Photodynamic Therapy. Journal of Chemical Information and Modeling, 2017, 57, 1089-1100.	5.4	17
57	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
58	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
59	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
60	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
61	The effect of Dâ€"[D_eâ€"Ïâ€"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
62	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
63	Theoretical investigation on the spectroscopic properties of furylfulgide with different substituents and design of novel bisâ€furylfulgimide photochromes. International Journal of Quantum Chemistry, 2017, 117, e25327.	2.0	1
64	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
65	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
66	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
67	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
68	Theoretical study of the cisâ€"trans isomerization mechanism of a pendant metal-bound azobenzene. RSC Advances, 2016, 6, 79879-79889.	3.6	8
69	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
70	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
71	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
72	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

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73	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
74	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
75	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
76	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
77	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
78	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
79	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
80	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
81	Molecular dynamics investigations of BioH protein substrate specificity for biotin synthesis. Journal of Biomolecular Structure and Dynamics, 2016, 34, 1052-1060.	3.5	6
82	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
83	Structural features and dynamic investigations of the membrane-bound cytochrome P450 17A1. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 2013-2021.	2.6	20
84	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
85	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
86	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
87	Investigation of ligand selectivity in CYP3A7 by molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2015, 33, 2360-2367.	3.5	19
88	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
89	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
90	Theoretical Investigation on Excited-State Cyclization Reactions of Platinum-Sensitized Dithienylethene Complexes. Journal of Physical Chemistry A, 2015, 119, 2819-2828.	2.5	11

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91	Theoretical studies on the spectroscopic properties of porphyrin derivatives for dye-sensitized solar cell application. RSC Advances, 2015, 5, 33653-33665.	3.6	30
92	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
93	Controllable molecular aggregation and fluorescence properties of 1,3,4-oxadiazole derivatives. Journal of Materials Chemistry C, 2015, 3, 11681-11688.	5.5	21
94	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
95	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
96	Theoretical evaluation and improvement on the potency of the rhodanine-based inhibitors for human serotoninN-acetyltransferase. Molecular Simulation, 2014, 40, 1201-1208.	2.0	1
97	Molecular simulation investigation on the interaction between barrier-to-autointegration factor dimer or its Gly25Glu mutant and LEM domain of emerin. Computational Biology and Chemistry, 2014, 53, 184-190.	2.3	1
98	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
99	Theoretical studies of the reaction of hydroxyl radical with cyclopentane (C5H10). Molecular Physics, 2014, 112, 963-971.	1.7	9
100	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
101	Theoretical study on the electronic structures and properties of diindolocarbazole isomers. Journal of Physical Organic Chemistry, 2014, 27, 973-980.	1.9	8
102	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
103	A theoretical analysis of the phosphorescence efficiencies of Cu(<scp>i</scp>) complexes. Dalton Transactions, 2014, 43, 11252-11259.	3.3	29
104	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
105	Design of Dâ€“Aâ€“Ïâ€“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
106	Theoretical study on molecular packing and electronic structure of bi-1,3,4-oxadiazole derivatives. RSC Advances, 2014, 4, 51942-51949.	3.6	7
107	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
108	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

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109	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
110	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
111	Theoretical study of gas phase reactions of important SOA intermediates: (cisâ€•and transâ€• BEPOX and Î²â€²EPOX with OH radical. International Journal of Quantum Chemistry, 2013, 113, 1162-1170.	2.0	0
112	Molecular dynamic studies on Langmuir monolayers of stearic acid. Chemical Research in Chinese Universities, 2013, 29, 545-550.	2.6	3
113	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
114	Theoretical analysis on magnetic properties of conjugated organic molecules containing borepin. Chemical Research in Chinese Universities, 2013, 29, 962-968.	2.6	3
115	Theoretical computation of lowâ€lying electronic states of HCNS: A CASPT2 study. International Journal of Quantum Chemistry, 2013, 113, 1416-1421.	2.0	1
116	Bisactinyl halogenated complexes: relativistic density functional theory calculation and experimental synthesis. RSC Advances, 2013, 3, 1572-1582.	3.6	8
117	Computational modelling of novel inhibitors targeting the human GSTP1*D homology domain. Molecular Simulation, 2013, 39, 550-562.	2.0	1
118	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
119	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
120	Drug Design Benefits from Molecular Dynamics: Some Examples. Current Computer-Aided Drug Design, 2013, 9, 532-546.	1.2	11
121	STABILITIES AND FRAGMENTATION BEHAVIORS OF Agn CLUSTERS (n = 2â€“34). Journal of Theoretical and Computational Chemistry, 2012, 11, 953-964.	1.8	8
122	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
123	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
124	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
125	Theoretical studies on the electronic structures and optical properties of the thiophene oligomer containing 2-(trifluoromethyl) thieno [3, 4-b] thiophene moiety and the CF3 end-caps. Journal of Polymer Research, 2012, 19, 1.	2.4	1
126	HOMOLOGY MODELING AND SUBSTRATE BINDING STUDY OF HUMAN KYNURENINE AMINOTRANSFERASE III. Journal of Theoretical and Computational Chemistry, 2012, 11, 855-870.	1.8	4

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127	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
128	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
129	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
130	Geometries and stabilities of Ag n v (vÂ=ÂÂ±1, 0; nÂ=Â21â€“29) clusters. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	9
131	Molecular Dynamics Simulations Suggest Ligandâ€™s Binding to Nicotinamidase/Pyrazinamidase. PLoS ONE, 2012, 7, e39546.	2.5	28
132	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. M Physics, 2011, 109, 645-653.	1.7	11
133	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
134	Low-lying electronic states of HNCS and its ions: a CASSCF/CASPT2 study. Theoretical Chemistry Accounts, 2011, 128, 215-222.	1.4	6
135	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
136	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
137	Theoretical Studies on Structures and Spectroscopic Properties of Highly Efficient Phosphorescent [Ru(terpy)(phen)X]+ Complexes. Chinese Journal of Chemical Physics, 2011, 24, 391-398.	1.3	0
138	Direct evidence for the effect of lateral hydrogen bonding on the smectic phase. Liquid Crystals, 2011, 38, 767-774.	2.2	15
139	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
140	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
141	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
142	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
143	Theoretical studies on the electronic structures and spectroscopic properties of a series of novel Nï£¿Cï£¿Nâ€coordinating Pt(II) complexes. International Journal of Quantum Chemistry, 2010, 110, 1605-1614.	2.0	1
144	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

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145	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
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