Likai Du

List of Publications by Year
in descending order

32 papers	565 citations	623734 14 h-index	642732 23 g-index
36 all docs	36 docs citations	36 times ranked	783 citing authors

#	Article	IF	Citations
1	Theoretical Study of the Oxidation of Methane to Methanol by the [CuIICuII(Î¼-O)2CuIII(7-N-Etppz)]1+ Complex. Inorganic Chemistry, 2018, 57, 3261-3271.	4.0	9
2	Charge-Transfer Knowledge Graph among Amino Acids Derived from High-Throughput Electronic Structure Calculations for Protein Database. ACS Omega, 2018, 3, 4094-4104.	3.5	8
3	Dioxygen Activation by Iron Complexes: The Catalytic Role of Intersystem Crossing Dynamics for a Heme-Related Model. Journal of Physical Chemistry C, 2018, 122, 2821-2831.	3.1	8
4	Computational Evidence for the Enzymatic Transformation of 2-Hydroxypropylphosphonate to Methylphosphonate. ACS Earth and Space Chemistry, 2018, 2, 888-894.	2.7	8
5	Spin crossover dynamics studies on the thermally activated molecular oxygen binding mechanism on a model copper complex. Physical Chemistry Chemical Physics, 2018, 20, 15852-15862.	2.8	2
6	How a single 5-methylation of cytosine regulates the recognition of C/EBPÎ² transcription factor: a molecular dynamic simulation study. Journal of Molecular Modeling, 2018, 24, 159.	1.8	6
7	Hydrogen bond dynamics governs the effective photoprotection mechanism of plant phenolic sunscreens. Photochemical and Photobiological Sciences, 2017, 16, 211-219.	2.9	16
8	Direct Learning Hidden Excited State Interaction Patterns from ab initio Dynamics and Its Implication as Alternative Molecular Mechanism Models. Scientific Reports, 2017, 7, 8737.	3.3	15
9	How Many Conformations of Enzymes Should Be Sampled for DFT/MM Calculations? A Case Study of Fluoroacetate Dehalogenase. International Journal of Molecular Sciences, 2016, 17, 1372.	4.1	16
10	Performance of density functional theory on the anisotropic halogenÂ·Â·Â·halogen interactions and potential energy surface: Problems and possible solutions. International Journal of Quantum Chemistry, 2016, 116, 710-717.	2.0	10
11	Atomic Resolution Insights into the Structural Aggregations and Optical Properties of Neat Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2016, 120, 6721-6729.	2.6	5
12	Ultrafast structural flattening motion in photoinduced excited state dynamics of a bis(diimine) copper(<scp>i</scp>) complex. Physical Chemistry Chemical Physics, 2016, 18, 7641-7650.	2.8	20
13	Catalytic mechanism of Câ€“F bond cleavage: insights from QM/MM analysis of fluoroacetate dehalogenase. Catalysis Science and Technology, 2016, 6, 73-80.	4.1	57
14	An On-the-Fly Surface-Hopping Program JADE for Nonadiabatic Molecular Dynamics of Polyatomic Systems: Implementation and Applications. Journal of Chemical Theory and Computation, 2015, 11, 1360-1374.	5.3	111
15	Photoinduced Ultrafast Intramolecular Excited-State Energy Transfer in the Silylene-Bridged Biphenyl and Stilbene (SBS) System: A Nonadiabatic Dynamics Point of View. Journal of Physical Chemistry A, 2015, 119, 6937-6948.	2.5	10
16	Application of polarizable ellipsoidal force field model to pnicogen bonds. Journal of Computational Chemistry, 2015, 36, 441-448.	3.3	13
17	Insights into the catalytic mechanism of chlorophenol 4-monooxygenase: a quantum mechanics/molecular mechanics study. RSC Advances, 2015, 5, 13871-13877.	3.6	11
18	Insight into the catalytic mechanism of meta-cleavage product hydrolase BphD: a quantum mechanics/molecular mechanics study. RSC Advances, 2015, 5, 66591-66597.	3.6	10

#	Article	IF	Citations
19	Photoinduced Excited-State Energy-Transfer Dynamics of a Nitrogen-Cored Symmetric Dendrimer: From the Perspective of the Jahnâ€“Teller Effect. Journal of Physical Chemistry C, 2015, 119, 7578-7589.	3.1	15
20	Theoretical study on the mechanism of selective fluorination of aromatic compounds with Selectfluor. RSC Advances, 2015, 5, 33385-33391.	3.6	22
21	Theoretical analysis of excited states and energy transfer mechanism in conjugated dendrimers. Journal of Computational Chemistry, 2015, 36, 151-163.	3.3	26
22	åŒ–å¦åŠ¨åŠ›å¦ä¸çš„éžç»›çƒè¿‡ç¨‹åŠå…¶ç†è®ºç”ç©¶. Scientia Sinica Chimica, 2015, 45, 777-799.	0.4	0
23	Polarization-enhanced bonding process of halogen bond, a theoretical study on Fâ€“H/Fâ€“X (X = F, Cl, Br,) Tj ETQq1 1 0.784314 rgBT /	1.9	3
24	A polarizable ellipsoidal force field for halogen bonds. Journal of Computational Chemistry, 2013, 34, 2032-2040.	3.3	28
25	THEORETICAL INVESTIGATION OF THE HIGH-SPIN "Fe-PROXIMAL OXYGEN" CATALYTIC MECHANISM OF RAT CYSTEINE DIOXYGENASE. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350001.	1.8	1
26	The reaction mechanism of hydroxyethylphosphonate dioxygenase: a QM/MM study. Organic and Biomolecular Chemistry, 2012, 10, 1014-1024.	2.8	19
27	Theoretical study on the aging and reactivation mechanism of tabun-inhibited acetylcholinesterase by using the quantum mechanicalâ€‰/â€‰molecular mechanical method. Canadian Journal of Chemistry, 2012, 90, 376-383.	1.1	6
28	Water-Dependent Reaction Pathways: An Essential Factor for the Catalysis in HEPD Enzyme. Journal of Physical Chemistry B, 2012, 116, 11837-11844.	2.6	22
29	QM/MM study on the spontaneous reactivation mechanism of (Â±)methamidophos-inhibited-acetylcholinesterase. Computational and Theoretical Chemistry, 2012, 980, 108-114.	2.5	9
30	A thermosensitive supramolecular aggregation from linear telechelic polydimethylsiloxane with self-assembly units. Journal of Polymer Research, 2011, 18, 1635-1643.	2.4	4
31	Glycosidic-Bond Hydrolysis Mechanism Catalyzed by Cellulase Cel7A from Trichoderma reesei: A Comprehensive Theoretical Study by Performing MD, QM, and QM/MM Calculations. Journal of Physical Chemistry B, 2010, 114, 15261-15268.	2.6	40
32	QM/MM Study on the Reaction Mechanism of O⁶-Alkylguanineâ^'DNA Alkyltransferase. Journal of Physical Chemistry B, 2010, 114, 15296-15300.	2.6	15