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	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
2	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
3	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
4	A polarizable ellipsoidal force field for halogen bonds. Journal of Computational Chemistry, 2013, 34, 2032-2040.	3.3	28
5	Theoretical analysis of excited states and energy transfer mechanism in conjugated dendrimers. Journal of Computational Chemistry, 2015, 36, 151-163.	3.3	26
6	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
7	Theoretical study on the mechanism of selective fluorination of aromatic compounds with Selectfluor. RSC Advances, 2015, 5, 33385-33391.	3.6	22
8	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
9	The reaction mechanism of hydroxyethylphosphonate dioxygenase: a QM/MM study. Organic and Biomolecular Chemistry, 2012, 10, 1014-1024.	2.8	19
10	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
11	Hydrogen bond dynamics governs the effective photoprotection mechanism of plant phenolic sunscreens. Photochemical and Photobiological Sciences, 2017, 16, 211-219.	2.9	16
12	QM/MM Study on the Reaction Mechanism of O⁶-Alkylguanineâ€"DNA Alkyltransferase. Journal of Physical Chemistry B, 2010, 114, 15296-15300.	2.6	15
13	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
14	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
15	Application of polarizable ellipsoidal force field model to pnicogen bonds. Journal of Computational Chemistry, 2015, 36, 441-448.	3.3	13
16	Insights into the catalytic mechanism of chlorophenol 4-monooxygenase: a quantum mechanics/molecular mechanics study. RSC Advances, 2015, 5, 13871-13877.	3.6	11
17	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
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	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
20	QM/MM study on the spontaneous reactivation mechanism of (Â±)methamidophos-inhibited-acetylcholinesterase. Computational and Theoretical Chemistry, 2012, 980, 108-114.	2.5	9
21	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
22	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
23	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
24	Computational Evidence for the Enzymatic Transformation of 2-Hydroxypropylphosphonate to Methylphosphonate. ACS Earth and Space Chemistry, 2018, 2, 888-894.	2.7	8
25	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
26	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
27	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
28	A thermosensitive supramolecular aggregation from linear telechelic polydimethylsiloxane with self-assembly units. Journal of Polymer Research, 2011, 18, 1635-1643.	2.4	4
29	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
30	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
31	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
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