Wen-Ge Han Du

List of Publications by Year
in descending order

36	1,758	279798 23	345221 36
papers	citations	h-index	g-index

37	37	37	1683
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum Chemical Studies of Intermediates and Reaction Pathways in Selected Enzymes and Catalytic Synthetic Systems. Chemical Reviews, 2004, 104, 459-508.	47.7	365
2	Structure, redox, pK a, spin. A golden tetrad for understanding metalloenzyme energetics and reaction pathways. Journal of Biological Inorganic Chemistry, 2006, 11, 674-694.	2.6	89
3	Sulfur [¹⁸F]Fluoride Exchange Click Chemistry Enabled Ultrafast Late-Stage Radiosynthesis. Journal of the American Chemical Society, 2021, 143, 3753-3763.	13.7	89
4	A Fluorogenic Aryl Fluorosulfate for Intraorganellar Transthyretin Imaging in Living Cells and in Caenorhabditis elegans. Journal of the American Chemical Society, 2015, 137, 7404-7414.	13.7	86
5	A Theoretical Study of the UV/Visible Absorption and Emission Solvatochromic Properties of Solvent-Sensitive Dyes. ChemPhysChem, 2003, 4, 1084-1094.	2.1	84
6	A Structural Model for the High-Valent Intermediate Q of Methane Monooxygenase from Broken-Symmetry Density Functional and Electrostatics Calculations. Journal of the American Chemical Society, 2002, 124, 5890-5894.	13.7	83
7	Density Functional Studies of the Ground- and Excited-State Potential-Energy Curves of Stilbenecis-trans Isomerization. ChemPhysChem, 2002, 3, 167-178.	2.1	75
8	Active Site Structure of Class I Ribonucleotide Reductase Intermediate X:Â A Density Functional Theory Analysis of Structure, Energetics, and Spectroscopy. Journal of the American Chemical Society, 2005, 127, 15778-15790.	13.7	70
9	Coupled Redox Potentials in Manganese and Iron Superoxide Dismutases from Reaction Kinetics and Density Functional/Electrostatics Calculations. Inorganic Chemistry, 2002, 41, 205-218.	4.0	69
10	DFT calculations of57Fe MÃ¶ssbauer isomer shifts and quadrupole splittings for iron complexes in polar dielectric media: Applications to methane monooxygenase and ribonucleotide reductase. Journal of Computational Chemistry, 2006, 27, 1292-1306.	3.3	61
11	Structural model studies for the high-valent intermediate Q of methane monooxygenase from broken-symmetry density functional calculations. Inorganica Chimica Acta, 2008, 361, 973-986.	2.4	61
12	Structural Model Studies for the Peroxo Intermediate P and the Reaction Pathway from P â†' Q of Methane Monooxygenase Using Broken-Symmetry Density Functional Calculations. Inorganic Chemistry, 2008, 47, 2975-2986.	4.0	58
13	Metal Substitution in the Active Site of Nitrogenase MFe7S9(M = Mo4+, V3+, Fe3+). Inorganic Chemistry, 2002, 41, 5744-5753.	4.0	53
14	DFT Calculations of Isomer Shifts and Quadrupole Splitting Parameters in Synthetic Ironâ^'Oxo Complexes:â€‰ Applications to Methane Monooxygenase and Ribonucleotide Reductase. Inorganic Chemistry, 2003, 42, 5244-5251.	4.0	47
15	Density Functional Vertical Self-Consistent Reaction Field Theory for Solvatochromism Studies of Solvent-Sensitive Dyes. Journal of Physical Chemistry A, 2004, 108, 3545-3555.	2.5	45
16	A Density Functional Evaluation of an Fe(III)â^'Fe(IV) Model Diiron Cluster:Â Comparisons with Ribonucleotide Reductase Intermediate X. Inorganic Chemistry, 2003, 42, 2751-2758.	4.0	41
17	Linking Chemical Electronâ€“Proton Transfer to Proton Pumping in Cytochrome c Oxidase: Broken-Symmetry DFT Exploration of Intermediates along the Catalytic Reaction Pathway of the Ironâ€“Copper Dinuclear Complex. Inorganic Chemistry, 2014, 53, 6458-6472.	4.0	38
18	Density Functional Theory Analysis of Structure, Energetics, and Spectroscopy for the Mnâ^'Fe Active Site of Chlamydia trachomatis Ribonucleotide Reductase in Four Oxidation States. Inorganic Chemistry, 2010, 49, 7266-7281.	4.0	32

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19	Geometric and Electrostatic Study of the [4Fe-4S] Cluster of Adenosine-5â€²-Phosphosulfate Reductase from Broken Symmetry Density Functional Calculations and Extended X-ray Absorption Fine Structure Spectroscopy. Inorganic Chemistry, 2011, 50, 6610-6625.	4.0	30
20	Seven clues to the origin and structure of class-I ribonucleotide reductase intermediate X. Journal of Inorganic Biochemistry, 2006, 100, 771-779.	3.5	29
21	DFT Calculations for Intermediate and Active States of the Diiron Center with a Tryptophan or Tyrosine Radical in Escherichia coli Ribonucleotide Reductase. Inorganic Chemistry, 2011, 50, 2302-2320.	4.0	26
22	Density Functional Study of a Î¼-1,1-Carboxylate Bridged Fe(III)â^'Oâ^'Fe(IV) Model Complex. 2. Comparison with Ribonucleotide Reductase Intermediate X. Inorganic Chemistry, 2004, 43, 613-621.	4.0	25
23	Experimental and DFT Studies:Â Novel Structural Modifications Greatly Enhance the Solvent Sensitivity of Live Cell Imaging Dyes. Journal of Physical Chemistry A, 2007, 111, 10849-10860.	2.5	25
24	Quantum cluster size and solvent polarity effects on the geometries and MÃ¶ssbauer properties of the active site model for ribonucleotide reductase intermediate X: a density functional theory study. Theoretical Chemistry Accounts, 2010, 125, 305-317.	1.4	23
25	Density Functional Study for the Bridged Dinuclear Center Based on a High-Resolution X-ray Crystal Structure of ba₃ Cytochrome c Oxidase from Thermus thermophilus. Inorganic Chemistry, 2013, 52, 14072-14088.	4.0	21
26	Broken Symmetry DFT Calculations/Analysis for Oxidized and Reduced Dinuclear Center in Cytochrome c Oxidase: Relating Structures, Protonation States, Energies, and MÃ¶ssbauer Properties in ba₃ Thermus thermophilus. Inorganic Chemistry, 2015, 54, 7272-7290.	4.0	21
27	A broken-symmetry density functional study of structures, energies, and protonation states along the catalytic Oâ€“O bond cleavage pathway in ba3 cytochrome c oxidase from Thermus thermophilus. Physical Chemistry Chemical Physics, 2016, 18, 21162-21171.	2.8	21
28	Water exit pathways and proton pumping mechanism in B-type cytochrome c oxidase from molecular dynamics simulations. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 1594-1606.	1.0	15
29	Data for molecular dynamics simulations of B-type cytochrome c oxidase with the Amber force field. Data in Brief, 2016, 8, 1209-1214.	1.0	13
30	Coupled transport of electrons and protons in a bacterial cytochromecoxidaseâ€”DFT calculated properties compared to structures and spectroscopies. Physical Chemistry Chemical Physics, 2020, 22, 26652-26668.	2.8	12
31	A Water Dimer Shift Activates a Proton Pumping Pathway in the P_R â†' F Transition of ba₃ Cytochrome c Oxidase. Inorganic Chemistry, 2018, 57, 1048-1059.	4.0	11
32	DFT Fe_{a3}â€“O/Oâ€“O Vibrational Frequency Calculations over Catalytic Reaction Cycle States in the Dinuclear Center of Cytochrome c Oxidase. Inorganic Chemistry, 2019, 58, 13933-13944.	4.0	11
33	Multiple reactive immunization towards the hydrolysis of organophosphorus nerve agents: hapten design and synthesis. Bioorganic and Medicinal Chemistry, 2001, 9, 3185-3195.	3.0	10
34	A Water Molecule Residing in the Fea33+Â·Â·Â·CuB2+Dinuclear Center of the Resting Oxidized as-Isolated CytochromecOxidase: A Density Functional Study. Inorganic Chemistry, 2020, 59, 8906-8915.	4.0	10
35	Temperature-Dependent Behavior of Protein-Chromophore Interactions: A Theoretical Study of a Blue Fluorescent Antibody. ChemPhysChem, 2003, 4, 848-855.	2.1	5
36	MÃ¶ssbauer Property Calculations on Fea33+â^™â^™â^™H2Oâ^™â^™â^™CuB2+ Dinuclear Center Models of the Resting Oxidized asâ€Isolated Cytochrome c Oxidase. ChemPhysChem, 2022, , .	2.1	2