

Wen-Ge Han Du

List of Publications by Year in descending order

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36
papers

1,758
citations

279798

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37
times ranked

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#	ARTICLE	IF	CITATIONS
1	MÃ¶ssbauer Property Calculations on Fea33+â™™â™™H2Oâ™™â™™CuB2+ Dinuclear Center Models of the Resting Oxidized as-Isolated Cytochrome c Oxidase. ChemPhysChem, 2022, , .	2.1	2
2	Sulfur [¹⁸ F]Fluoride Exchange Click Chemistry Enabled Ultrafast Late-Stage Radiosynthesis. Journal of the American Chemical Society, 2021, 143, 3753-3763.	13.7	89
3	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
4	A Water Molecule Residing in the Fea33+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
5	DFT Fe_{a3}â€™O/Oâ€™O Vibrational Frequency Calculations over Catalytic Reaction Cycle States in the Dinuclear Center of Cytochrome <i>c</i> Oxidase. Inorganic Chemistry, 2019, 58, 13933-13944.	4.0	11
6	A Water Dimer Shift Activates a Proton Pumping Pathway in the P_{R} â†’ F Transition of <i>ba</i>₃ Cytochrome <i>c</i> Oxidase. Inorganic Chemistry, 2018, 57, 1048-1059.	4.0	11
7	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
8	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
9	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
10	A Fluorogenic Aryl Fluorosulfate for Intraorganellar Transthyretin Imaging in Living Cells and in <i>Caenorhabditis elegans</i>. Journal of the American Chemical Society, 2015, 137, 7404-7414.	13.7	86
11	Broken Symmetry DFT Calculations/Analysis for Oxidized and Reduced Dinuclear Center in Cytochrome <i>c</i> Oxidase: Relating Structures, Protonation States, Energies, and MÃ¶ssbauer Properties in <i>ba</i>₃ <i>Thermus thermophilus</i>. Inorganic Chemistry, 2015, 54, 7272-7290.	4.0	21
12	Linking Chemical Electronâ€™Proton Transfer to Proton Pumping in Cytochrome <i>c</i> 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
13	Density Functional Study for the Bridged Dinuclear Center Based on a High-Resolution X-ray Crystal Structure of <i>ba</i>₃ Cytochrome <i>c</i> Oxidase from Thermus thermophilus. Inorganic Chemistry, 2013, 52, 14072-14088.	4.0	21
14	DFT Calculations for Intermediate and Active States of the Diiron Center with a Tryptophan or Tyrosine Radical in <i>Escherichia coli</i> Ribonucleotide Reductase. Inorganic Chemistry, 2011, 50, 2302-2320.	4.0	26
15	Geometric and Electrostatic Study of the [4Fe-4S] Cluster of Adenosine-5â€™-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
16	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
17	Density Functional Theory Analysis of Structure, Energetics, and Spectroscopy for the Mnâ€™Fe Active Site of <i>Chlamydia trachomatis</i> Ribonucleotide Reductase in Four Oxidation States. Inorganic Chemistry, 2010, 49, 7266-7281.	4.0	32
18	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

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19	Structural Model Studies for the Peroxo Intermediate P and the Reaction Pathway from P to Q of Methane Monooxygenase Using Broken-Symmetry Density Functional Calculations. <i>Inorganic Chemistry</i> , 2008, 47, 2975-2986.	4.0	58
20	Experimental and DFT Studies: Novel Structural Modifications Greatly Enhance the Solvent Sensitivity of Live Cell Imaging Dyes. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10849-10860.	2.5	25
21	Structure, redox, pK _a , spin. A golden tetrad for understanding metalloenzyme energetics and reaction pathways. <i>Journal of Biological Inorganic Chemistry</i> , 2006, 11, 674-694.	2.6	89
22	Seven clues to the origin and structure of class-I ribonucleotide reductase intermediate X. <i>Journal of Inorganic Biochemistry</i> , 2006, 100, 771-779.	3.5	29
23	DFT calculations of ⁵⁷ Fe Mössbauer isomer shifts and quadrupole splittings for iron complexes in polar dielectric media: Applications to methane monooxygenase and ribonucleotide reductase. <i>Journal of Computational Chemistry</i> , 2006, 27, 1292-1306.	3.3	61
24	Active Site Structure of Class I Ribonucleotide Reductase Intermediate X: A Density Functional Theory Analysis of Structure, Energetics, and Spectroscopy. <i>Journal of the American Chemical Society</i> , 2005, 127, 15778-15790.	13.7	70
25	Density Functional Study of a μ_2 -1,1-Carboxylate Bridged Fe(III)-O-Fe(IV) Model Complex. 2. Comparison with Ribonucleotide Reductase Intermediate X. <i>Inorganic Chemistry</i> , 2004, 43, 613-621.	4.0	25
26	Quantum Chemical Studies of Intermediates and Reaction Pathways in Selected Enzymes and Catalytic Synthetic Systems. <i>Chemical Reviews</i> , 2004, 104, 459-508.	47.7	365
27	Density Functional Vertical Self-Consistent Reaction Field Theory for Solvatochromism Studies of Solvent-Sensitive Dyes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3545-3555.	2.5	45
28	Temperature-Dependent Behavior of Protein-Chromophore Interactions: A Theoretical Study of a Blue Fluorescent Antibody. <i>ChemPhysChem</i> , 2003, 4, 848-855.	2.1	5
29	A Theoretical Study of the UV/Visible Absorption and Emission Solvatochromic Properties of Solvent-Sensitive Dyes. <i>ChemPhysChem</i> , 2003, 4, 1084-1094.	2.1	84
30	A Density Functional Evaluation of an Fe(III)-Fe(IV) Model Diiron Cluster: Comparisons with Ribonucleotide Reductase Intermediate X. <i>Inorganic Chemistry</i> , 2003, 42, 2751-2758.	4.0	41
31	DFT Calculations of Isomer Shifts and Quadrupole Splitting Parameters in Synthetic Iron-Oxo Complexes: Applications to Methane Monooxygenase and Ribonucleotide Reductase. <i>Inorganic Chemistry</i> , 2003, 42, 5244-5251.	4.0	47
32	A Structural Model for the High-Valent Intermediate Q of Methane Monooxygenase from Broken-Symmetry Density Functional and Electrostatics Calculations. <i>Journal of the American Chemical Society</i> , 2002, 124, 5890-5894.	13.7	83
33	Coupled Redox Potentials in Manganese and Iron Superoxide Dismutases from Reaction Kinetics and Density Functional/Electrostatics Calculations. <i>Inorganic Chemistry</i> , 2002, 41, 205-218.	4.0	69
34	Metal Substitution in the Active Site of Nitrogenase MFe ₇ S ₉ (M = Mo ⁴⁺ , V ³⁺ , Fe ³⁺). <i>Inorganic Chemistry</i> , 2002, 41, 5744-5753.	4.0	53
35	Density Functional Studies of the Ground- and Excited-State Potential-Energy Curves of Stilbenecis-trans Isomerization. <i>ChemPhysChem</i> , 2002, 3, 167-178.	2.1	75
36	Multiple reactive immunization towards the hydrolysis of organophosphorus nerve agents: hapten design and synthesis. <i>Bioorganic and Medicinal Chemistry</i> , 2001, 9, 3185-3195.	3.0	10