Kyung-Bin Cho

List of Publications by Year
in descending order

81 papers	3,793 citations	87888 38 h-index	133252 59 g-index
85 all docs	85 docs citations	85 times ranked	2740 citing authors

#	Article	IF	Citations
1	A Highly Reactive Mononuclear Non-Heme Manganese(IV)â€"Oxo Complex That Can Activate the Strong Câ€"H Bonds of Alkanes. Journal of the American Chemical Society, 2011, 133, 20088-20091.	13.7	198
2	A Mononuclear Non-Heme Manganese(IV)â€"Oxo Complex Binding Redox-Inactive Metal Ions. Journal of the American Chemical Society, 2013, 135, 6388-6391.	13.7	182
3	A mononuclear nonheme iron(iv)-oxo complex which is more reactive than cytochrome P450 model compound I. Chemical Science, 2011, 2, 1039.	7.4	170
4	To rebound or dissociate? This is the mechanistic question in Câ€"H hydroxylation by heme and nonheme metalâ€"oxo complexes. Chemical Society Reviews, 2016, 45, 1197-1210.	38.1	167
5	Evidence for an Alternative to the Oxygen Rebound Mechanism in Câ€"H Bond Activation by Non-Heme Fe^{IV}O Complexes. Journal of the American Chemical Society, 2012, 134, 20222-20225.	13.7	137
6	Redox-inactive metal ions modulate the reactivity and oxygen release of mononuclear non-haem iron(III)â€"peroxo complexes. Nature Chemistry, 2014, 6, 934-940.	13.6	135
7	Synthesis and reactivity of a mononuclear non-haem cobalt(IV)-oxo complex. Nature Communications, 2017, 8, 14839.	12.8	132
8	Enhanced Electron-Transfer Reactivity of Nonheme Manganese(IV)â€"Oxo Complexes by Binding Scandium Ions. Journal of the American Chemical Society, 2013, 135, 9186-9194.	13.7	131
9	A Manganese(V)â€"Oxo Complex: Synthesis by Dioxygen Activation and Enhancement of Its Oxidizing Power by Binding Scandium Ion. Journal of the American Chemical Society, 2016, 138, 8523-8532.	13.7	118
10	Ligand Topology Effect on the Reactivity of a Mononuclear Nonheme Iron(IV)-Oxo Complex in Oxygenation Reactions. Journal of the American Chemical Society, 2011, 133, 11876-11879.	13.7	94
11	Water as an Oxygen Source: Synthesis, Characterization, and Reactivity Studies of a Mononuclear Nonheme Manganese(IV) Oxo Complex. Angewandte Chemie - International Edition, 2010, 49, 8190-8194.	13.8	90
12	Interplay of Experiment and Theory in Elucidating Mechanisms of Oxidation Reactions by a Nonheme Ru^{IV}O Complex. Journal of the American Chemical Society, 2015, 137, 8623-8632.	13.7	85
13	Theoretical Investigations into Câ€"H Bond Activation Reaction by Nonheme Mn^{IV}O Complexes: Multistate Reactivity with No Oxygen Rebound. Journal of Physical Chemistry Letters, 2012, 3, 2851-2856.	4.6	77
14	External Electric Field Can Control the Catalytic Cycle of Cytochrome P450_{cam}: A QM/MM Study. Journal of Physical Chemistry Letters, 2010, 1, 2082-2087.	4.6	76
15	A Mononuclear Non-Heme High-Spin Iron(III)â€"Hydroperoxo Complex as an Active Oxidant in Sulfoxidation Reactions. Journal of the American Chemical Society, 2013, 135, 8838-8841.	13.7	71
16	Oxidation of Tertiary Amines by Cytochrome P450â€"Kinetic Isotope Effect as a Spinâ€State Reactivity Probe. Chemistry - A European Journal, 2009, 15, 8492-8503.	3.3	68
17	Mechanistic insight into the hydroxylation of alkanes by a nonheme iron(<scp>v</scp>)â€"oxo complex. Chemical Communications, 2014, 50, 5572-5575.	4.1	67
18	Dioxygen Activation by a Non-Heme Iron(II) Complex: Theoretical Study toward Understanding Ferricâ€"Superoxo Complexes. Journal of Chemical Theory and Computation, 2012, 8, 915-926.	5.3	65

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19	Determination of Spin Inversion Probability, H-Tunneling Correction, and Regioselectivity in the Two-State Reactivity of Nonheme Iron(IV)-Oxo Complexes. Journal of Physical Chemistry Letters, 2015, 6, 1472-1476.	4.6	64
20	Reactivity comparison of high-valent iron(iv)-oxo complexes bearing N-tetramethylated cyclam ligands with different ring size. Dalton Transactions, 2013, 42, 7842.	3.3	61
21	Mechanistic dichotomies in redox reactions of mononuclear metalâ€“oxygen intermediates. Chemical Society Reviews, 2020, 49, 8988-9027.	38.1	61
22	Compound I of Nitric Oxide Synthase:Â The Active Site Protonation State. Journal of the American Chemical Society, 2007, 129, 3182-3188.	13.7	59
23	Mechanistic Insights into the Câ€“H Bond Activation of Hydrocarbons by Chromium(IV) Oxo and Chromium(III) Superoxo Complexes. Inorganic Chemistry, 2014, 53, 645-652.	4.0	52
24	Factors Controlling the Chemoselectivity in the Oxidation of Olefins by Nonheme Manganese(IV)-Oxo Complexes. Journal of the American Chemical Society, 2016, 138, 10654-10663.	13.7	52
25	Demonstration of the Heterolytic Oï£¿O Bond Cleavage of Putative Nonheme Iron(II)ï£¿OOH(R) Complexes for Fenton and Enzymatic Reactions. Angewandte Chemie - International Edition, 2014, 53, 7843-7847.	13.8	50
26	Reactions of a Chromium(III)-Superoxo Complex and Nitric Oxide That Lead to the Formation of Chromium(IV)-Oxo and Chromium(III)-Nitrito Complexes. Journal of the American Chemical Society, 2013, 135, 14900-14903.	13.7	49
27	Spectroscopic Characterization and Reactivity Studies of a Mononuclear Nonheme Mn(III)â€“Hydroperoxo Complex. Journal of the American Chemical Society, 2014, 136, 12229-12232.	13.7	49
28	Formation of the Active Species of Cytochromeâ€...P450 by Using Iodosylbenzene: A Case for Spin-Selective Reactivity. Chemistry - A European Journal, 2007, 13, 4103-4115.	3.3	46
29	Conversion of high-spin iron(<scp>iii</scp>)â€“alkylperoxo to iron(<scp>iv</scp>)â€“oxo species via Oâ€“O bond homolysis in nonheme iron models. Chemical Science, 2014, 5, 156-162.	7.4	46
30	Mononuclear Nonheme Highâ€Spin (<i>S</i>=2) versus Intermediateâ€Spin (<i>S</i>=1) Iron(IV)â€“Oxo Complexes in Oxidation Reactions. Angewandte Chemie - International Edition, 2016, 55, 8027-8031.	13.8	46
31	High-Spin Mn(V)-Oxo Intermediate in Nonheme Manganese Complex-Catalyzed Alkane Hydroxylation Reaction: Experimental and Theoretical Approach. Inorganic Chemistry, 2019, 58, 14842-14852.	4.0	46
32	Mononuclear Manganeseâ€“Peroxo and Bis(Î¼â€oxo)dimanganese Complexes Bearing a Common Nâ€Methylated Macrocyclic Ligand. Chemistry - A European Journal, 2013, 19, 14119-14125.	3.3	44
33	A mononuclear manganese(<scp>iii</scp>)â€“hydroperoxo complex: synthesis by activating dioxygen and reactivity in electrophilic and nucleophilic reactions. Chemical Communications, 2018, 54, 1209-1212.	4.1	43
34	Electron-Transfer and Redox Reactivity of High-Valent Iron Imido and Oxo Complexes with the Formal Oxidation States of Five and Six. Journal of the American Chemical Society, 2020, 142, 3891-3904.	13.7	43
35	Mononuclear nonheme iron(<scp>iv</scp>)â€“oxo and manganese(<scp>iv</scp>)â€“oxo complexes in oxidation reactions: experimental results prove theoretical prediction. Chemical Communications, 2015, 51, 13094-13097.	4.1	42
36	The Fe^{III}(H₂O₂) Complex as a Highly Efficient Oxidant in Sulfoxidation Reactions: Revival of an Underrated Oxidant in Cytochrome P450. Journal of Chemical Theory and Computation, 2013, 9, 2519-2525.	5.3	41

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37	First Half-Reaction Mechanism of Nitric Oxide Synthase: The Role of Proton and Oxygen Coupled Electron Transfer in the Reaction by Quantum Mechanics/Molecular Mechanics. Journal of Physical Chemistry B, 2009, 113, 336-346.	2.6	40
38	Mutable Properties of Nonheme Iron(III)â€“Iodosylarene Complexes Result in the Elusive Multiple-Oxidant Mechanism. Journal of the American Chemical Society, 2017, 139, 7444-7447.	13.7	40
39	Spectroscopic and computational characterization of CuIIâ€“OOR (R = H or cumyl) complexes bearing a Me6-tren ligand. Dalton Transactions, 2011, 40, 2234.	3.3	39
40	Nonheme iron-oxo and -superoxo reactivities: O2 binding and spin inversion probability matter. Chemical Communications, 2012, 48, 2189.	4.1	39
41	New Trans-Chelating Ligands and Their Complexes and Catalytic Properties in the Mizorokiâˆ'Heck Arylation of Cyclohexene. Organometallics, 2008, 27, 5139-5145.	2.3	38
42	Influence of Cu+on the RSâˆ'NO Bond Dissociation Energy of S-Nitrosothiols. Journal of Physical Chemistry B, 2005, 109, 1334-1336.	2.6	34
43	Compound I in Heme Thiolate Enzymes: A Comparative QM/MM Study. Journal of Physical Chemistry A, 2008, 112, 13128-13138.	2.5	32
44	Class I ribonucleotide reductase revisited: The effect of removing a proton on Glu441. Journal of Computational Chemistry, 2004, 25, 311-321.	3.3	31
45	A Density Functional Theory Investigation on the Mechanism of the Second Half-Reaction of Nitric Oxide Synthase. Journal of the American Chemical Society, 2008, 130, 3328-3334.	13.7	30
46	Second Half-Reaction of Nitric Oxide Synthase:â€‰ Computational Insights into the Initial Step and Key Proposed Intermediate. Journal of Physical Chemistry B, 2005, 109, 23706-23714.	2.6	28
47	Effects of Substrate, Protein Environment, and Proximal Ligand Mutation on Compound I and Compound 0 of Chloroperoxidase. Journal of Physical Chemistry A, 2009, 113, 11763-11771.	2.5	26
48	A mononuclear nonheme cobalt(<scp>iii</scp>)â€“hydroperoxide complex with an amphoteric reactivity in electrophilic and nucleophilic oxidative reactions. Dalton Transactions, 2016, 45, 14511-14515.	3.3	26
49	Structure and spin state of nonheme Fe^{IV}O complexes depending on temperature: predictive insights from DFT calculations and experiments. Chemical Science, 2017, 8, 5460-5467.	7.4	25
50	Correlating DFTâ€Calculated Energy Barriers to Experiments in Nonheme Octahedral Fe^{IV}O Species. Chemistry - A European Journal, 2012, 18, 10444-10453.	3.3	24
51	Theoretical predictions of a highly reactive non-heme Fe(iv)î€O complex with a high-spin ground state. Chemical Communications, 2010, 46, 4511.	4.1	23
52	Mechanistic Insight into the Nitric Oxide Dioxygenation Reaction of Nonheme Iron(III)â€“Superoxo and Manganese(IV)â€“Peroxo Complexes. Angewandte Chemie - International Edition, 2016, 55, 12403-12407.	13.8	23
53	Tunneling Effect That Changes the Reaction Pathway from Epoxidation to Hydroxylation in the Oxidation of Cyclohexene by a Compound I Model of Cytochrome P450. Journal of Physical Chemistry Letters, 2017, 8, 1557-1561.	4.6	23
54	Tuning the Reactivity of Chromium(III)-Superoxo Species by Coordinating Axial Ligands. Inorganic Chemistry, 2015, 54, 10513-10520.	4.0	21

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55	The Substrate Reaction Mechanism of Class III Anaerobic Ribonucleotide Reductase. Journal of Physical Chemistry B, 2001, 105, 6445-6452.	2.6	19
56	Quantum Chemical Calculations of the NHA Bound Nitric Oxide Synthase Active Site:Â O2Binding and Implications for the Catalytic Mechanism. Journal of the American Chemical Society, 2004, 126, 10267-10270.	13.7	18
57	The reaction mechanism of allene oxide synthase: Interplay of theoretical QM/MM calculations and experimental investigations. Archives of Biochemistry and Biophysics, 2011, 507, 14-25.	3.0	17
58	Bromoacetic Acid-Promoted Nonheme Manganese-Catalyzed Alkane Hydroxylation Inspired by Î±-Ketoglutarate-Dependent Oxygenases. ACS Catalysis, 2022, 12, 6756-6769.	11.2	17
59	Tuning the Redox Properties of a Nonheme Iron(III)â€"Peroxo Complex Binding Redoxâ€Inactive Zinc Ions by Water Molecules. Chemistry - A European Journal, 2015, 21, 10676-10680.	3.3	14
60	Density Functional Calculations on Class III Ribonucleotide Reductase:Â Substrate Reaction Mechanism with Two Formates. Journal of Physical Chemistry B, 2004, 108, 2056-2065.	2.6	13
61	A Computational Study on the Interaction of the Nitric Oxide Ions NO+ and NO- with the Side Groups of the Aromatic Amino Acids. Journal of Physical Chemistry A, 2007, 111, 1981-1989.	2.5	13
62	A theoretical study into a trans-dioxo Mn^V porphyrin complex that does not follow the oxygen rebound mechanism in Câ€"H bond activation reactions. Chemical Communications, 2016, 52, 904-907.	4.1	13
63	Mononuclear Nonheme Highâ€Spin (<i>S</i>=2) versus Intermediateâ€Spin (<i>S</i>=1) Iron(IV)â€"Oxo Complexes in Oxidation Reactions. Angewandte Chemie, 2016, 128, 8159-8163.	2.0	12
64	A theoretical investigation into the first-row transition metalâ€"O₂adducts. Inorganic Chemistry Frontiers, 2019, 6, 2071-2081.	6.0	12
65	QM/MM theoretical study of the pentacoordinate Mn(III) and resting states of manganese-reconstituted cytochrome P450cam. Journal of Biological Inorganic Chemistry, 2008, 13, 521-530.	2.6	10
66	Electronic properties and reactivity patterns of <scp>highâ€valent metalâ€oxo</scp> species of Mn, Fe, Co, and Ni. Bulletin of the Korean Chemical Society, 2021, 42, 1506-1512.	1.9	9
67	Metalâ€"ligand cooperative transformation of alkyl azide to isocyanate occurring at a Coâ€"Si moiety. Chemical Communications, 2021, 57, 3219-3222.	4.1	8
68	Heme compound II models in chemoselectivity and disproportionation reactions. Chemical Science, 0, , .	7.4	8
69	Investigating Superoxide Transfer through a Î¼-1,2-O₂ Bridge between Nonheme Ni^{III}â€"Peroxo and Mn^{II} Species by DFT Methods to Bridge Theoretical and Experimental Views. Journal of Physical Chemistry Letters, 2014, 5, 2437-2442.	4.6	7
70	Ligand Architecture Perturbation Influences the Reactivity of Nonheme Iron(V)-Oxo Tetraamido Macrocyclic Ligand Complexes: A Combined Experimental and Theoretical Study. Inorganic Chemistry, 2021, 60, 4058-4067.	4.0	7
71	Peroxyl adduct radicals formed in the iron/oxygen reconstitution reaction of mutant ribonucleotide reductase R2 proteins from Escherichia coli. Journal of Biological Inorganic Chemistry, 2002, 7, 74-82.	2.6	6
72	Conformations of Benzene- and Dibenzo[a,l]pyrene Diol Epoxides Studied by Density Functional Theory:â€‰ Ground States, Transition States, Dynamics, and Solvent Effects. Chemical Research in Toxicology, 2003, 16, 590-597.	3.3	6

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73	Nickel-Catalyzed NO Group Transfer Coupled with NO_{<i>x</i>} Conversion. Journal of the American Chemical Society, 2022, 144, 4585-4593.	13.7	6
74	Structure and Reactivity of Nonporphyrinic Terminal Manganese(IV)â€“Hydroxide Complexes in the Oxidative Electrophilic Reaction. Inorganic Chemistry, 2022, 61, 4292-4301.	4.0	6
75	Mechanistic Insight into the Nitric Oxide Dioxygenation Reaction of Nonheme Iron(III)â€“Superoxo and Manganese(IV)â€“Peroxo Complexes. Angewandte Chemie, 2016, 128, 12591-12595.	2.0	5
76	How does Lewis acid affect the reactivity of mononuclear <scp>highâ€valent chromiumâ€“oxo</scp> species? A theoretical study. Bulletin of the Korean Chemical Society, 2021, 42, 1501-1505.	1.9	5
77	Ring Complexes of S-Nitrosothiols with Cu+: A Density Functional Theory Study. European Journal of Mass Spectrometry, 2004, 10, 941-948.	1.0	4
78	Intermetal oxygen atom transfer from an Fe^VO complex to a Mn^{III} complex: an experimental and theoretical approach. Chemical Communications, 2016, 52, 12968-12971.	4.1	4
79	Nonheme Iron Imido Complexes Bearing a Nonâ€Innocent Ligand: A Synthetic Chameleon Species in Oxidation Reactions. Chemistry - A European Journal, 2021, 27, 17495-17503.	3.3	2
80	Mono- and dinuclear zinc complexes bearing identical bis(thiosemicarbazone) ligand that exhibit alkaline phosphatase-like catalytic reactivity. Journal of Biological Inorganic Chemistry, 2021, , 1.	2.6	1
81	An end-on bis(Î¼-hydroxido) dimanganese(<scp>ii</scp>,<scp>iii</scp>) azide complex for Câ€“H bond and Oâ€“H bond activation reactions. Chemical Communications, 2022, 58, 4623-4626.	4.1	1