Abhishek Dey

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6781855/publications.pdf

Version: 2024-02-01

161	7,045	41323 49	74108 75
papers	citations	h-index	g-index

169	169	169	5842
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	O₂ reduction by iron porphyrins with electron withdrawing groups: to scale or not to scale. Faraday Discussions, 2022, 234, 143-158.	1.6	7
2	Synthetic heme dioxygen adducts: electronic structure and reactivity. Trends in Chemistry, 2022, 4, 15-31.	4.4	3
3	Selectivity in Electrochemical CO₂ Reduction. Accounts of Chemical Research, 2022, 55, 134-144.	7.6	152
4	A Bidirectional Bioinspired [FeFe]-Hydrogenase Model. Journal of the American Chemical Society, 2022, 144, 3614-3625.	6.6	31
5	Assembly of redox active metallo-enzymes and metallo-peptides on electrodes: Abiological constructs to probe natural processes. Current Opinion in Chemical Biology, 2022, 68, 102142.	2.8	2
6	Recent developments in the synthesis of bio-inspired iron porphyrins for small molecule activation. Chemical Communications, 2022, 58, 5808-5828.	2.2	9
7	Second Sphere Effects on Oxygen Reduction and Peroxide Activation by Mononuclear Iron Porphyrins and Related Systems. Chemical Reviews, 2022, 122, 12370-12426.	23.0	44
8	Bioinorganic Chemistry on Electrodes: Methods to Functional Modeling. Journal of the American Chemical Society, 2022, 144, 8402-8429.	6.6	7
9	Electrocatalytic Water Oxidation by a Phosphorusâ€“Nitrogen Oâ•PN3-Pincer Cobalt Complex. Inorganic Chemistry, 2021, 60, 614-622.	1.9	14
10	Intermediates involved in serotonin oxidation catalyzed by Cu bound AÎ² peptides. Chemical Science, 2021, 12, 1924-1929.	3.7	11
11	Introduction to (photo)electrocatalysis for renewable energy. Chemical Communications, 2021, 57, 1540-1542.	2.2	3
12	Biochemical and artificial pathways for the reduction of carbon dioxide, nitrite and the competing proton reduction: effect of 2ndsphere interactions in catalysis. Chemical Society Reviews, 2021, 50, 3755-3823.	18.7	77
13	Contributions to cytochrome <i>c</i> inner- and outer-sphere reorganization energy. Chemical Science, 2021, 12, 11894-11913.	3.7	9
14	An [FeFe]â€Hydrogenase Mimic Immobilized through Simple Physiadsorption and Active for Aqueous H₂ Production. ChemElectroChem, 2021, 8, 1674-1677.	1.7	9
15	Proton Relay in Iron Porphyrins for Hydrogen Evolution Reaction. Inorganic Chemistry, 2021, 60, 13876-13887.	1.9	26
16	Ligand Radical Mediated Water Oxidation by a Family of Copper <i>o</i>-Phenylene Bis-oxamidate Complexes. Inorganic Chemistry, 2021, 60, 9442-9455.	1.9	18
17	Proton reduction in the presence of oxygen by iron porphyrin enabled with 2nd sphere redox active ferrocenes. Chinese Journal of Catalysis, 2021, 42, 1327-1331.	6.9	7
18	Activating the Fe(I) State of Iron Porphyrinoid with Second-Sphere Proton Transfer Residues for Selective Reduction of CO₂ to HCOOH via Fe(III/II)â€“COOH Intermediate(s). Journal of the American Chemical Society, 2021, 143, 13579-13592.	6.6	59

#	Article	IF	Citations
19	Rejigging Electron and Proton Transfer to Transition between Dioxygenase, Monooxygenase, Peroxygenase, and Oxygen Reduction Activity: Insights from Bioinspired Constructs of Heme Enzymes. Jacs Au, 2021, 1, 1296-1311.	3.6	10
20	Kinetic Isotope Effects on Electron Transfer Across Self-Assembled Monolayers on Gold. Inorganic Chemistry, 2021, 60, 597-605.	1.9	7
21	A Single Iron Porphyrin Shows pH Dependent Switch between â€œPushâ€•and â€œPullâ€•Effects in Electrochemical Oxygen Reduction. Inorganic Chemistry, 2020, 59, 14564-14576.	1.9	12
22	Electrocatalytic Reduction of Nitrogen to Hydrazine Using a Trinuclear Nickel Complex. Journal of the American Chemical Society, 2020, 142, 17312-17317.	6.6	41
23	Elucidation of Factors That Govern the 2e^{â€“}/2H⁺ vs 4e^{â€“}/4H⁺ Selectivity of Water Oxidation by a Cobalt Corrole. Journal of the American Chemical Society, 2020, 142, 21040-21049.	6.6	44
24	Nano-Apples and Orange-Zymes. ACS Catalysis, 2020, 10, 14315-14317.	5.5	33
25	Repurposing a Bio-Inspired NiFe Hydrogenase Model for CO₂ Reduction with Selective Production of Methane as the Unique C-Based Product. ACS Energy Letters, 2020, 5, 3837-3842.	8.8	41
26	Effect of Pendant Distal Residues on the Rate and Selectivity of Electrochemical Oxygen Reduction Reaction Catalyzed by Iron Porphyrin Complexes. ACS Catalysis, 2020, 10, 13136-13148.	5.5	30
27	A heterogeneous bio-inspired peroxide shunt for catalytic oxidation of organic molecules. Chemical Communications, 2020, 56, 11593-11596.	2.2	8
28	Oxygen Reduction by Iron Porphyrins with Covalently Attached Pendent Phenol and Quinol. Journal of the American Chemical Society, 2020, 142, 21810-21828.	6.6	38
29	Organic Electrosynthesis: When Is It Electrocatalysis?. ACS Catalysis, 2020, 10, 13156-13158.	5.5	26
30	Catalytic Câ€“H Bond Oxidation Using Dioxygen by Analogues of Heme Superoxide. Inorganic Chemistry, 2020, 59, 7415-7425.	1.9	13
31	The role of porphyrin peripheral substituents in determining the reactivities of ferrous nitrosyl species. Chemical Science, 2020, 11, 5909-5921.	3.7	16
32	Excellence <i>versus</i> Diversity? Not an Either/Or Choice. ACS Catalysis, 2020, 10, 7310-7311.	5.5	4
33	A designed second-sphere hydrogen-bond interaction that critically influences the Oâ€“O bond activation for heterolytic cleavage in ferric ironâ€“porphyrin complexes. Chemical Science, 2020, 11, 2681-2695.	3.7	24
34	Homogeneous Electrochemical Reduction of CO₂ to CO by a Cobalt Pyridine Thiolate Complex. Inorganic Chemistry, 2020, 59, 5292-5302.	1.9	30
35	Formation of compound I in heme bound AÎ²-peptides relevant to Alzheimer's disease. Chemical Science, 2019, 10, 8405-8410.	3.7	14
36	Resonance Raman Spectroscopy and Density Functional Theory Calculations on Ferrous Porphyrin Dioxygen Adducts with Different Axial Ligands: Correlation of Ground State Wave Function and Geometric Parameters with Experimental Vibrational Frequencies. Inorganic Chemistry, 2019, 58, 10704-10715.	1.9	13

#	ARTICLE	IF	CITATIONS
37	Influence of the distal guanidine group on the rate and selectivity of O₂ reduction by iron porphyrin. Chemical Science, 2019, 10, 9692-9698.	3.7	33
38	Role of 2nd sphere H-bonding residues in tuning the kinetics of CO₂ reduction to CO by iron porphyrin complexes. Dalton Transactions, 2019, 48, 5965-5977.	1.6	74
39	Effect of hydrogen bonding on innocent and non-innocent axial ligands bound to iron porphyrins. Dalton Transactions, 2019, 48, 7179-7186.	1.6	14
40	Recent developments in bioinspired modelling of [NiFe]- and [FeFe]-hydrogenases. Current Opinion in Electrochemistry, 2019, 15, 155-164.	2.5	34
41	A bi-functional cobalt-porphyrinoid electrocatalyst: balance between overpotential and selectivity. Journal of Biological Inorganic Chemistry, 2019, 24, 437-442.	1.1	8
42	Formally Ferric Heme Carbon Monoxide Adduct. Journal of the American Chemical Society, 2019, 141, 5073-5077.	6.6	6
43	Hydrogen atom abstraction by synthetic heme ferric superoxide and hydroperoxide species. Chemical Communications, 2019, 55, 5591-5594.	2.2	19
44	Reduction of CO₂ to CO by an Iron Porphyrin Catalyst in the Presence of Oxygen. ACS Catalysis, 2019, 9, 3895-3899.	5.5	68
45	Electron Transfer Control of Reductase versus Monooxygenase: Catalytic Câ€“H Bond Hydroxylation and Alkene Epoxidation by Molecular Oxygen. ACS Central Science, 2019, 5, 671-682.	5.3	47
46	Tailor made iron porphyrins for investigating axial ligand and distal environment contributions to electronic structure and reactivity. Coordination Chemistry Reviews, 2019, 386, 183-208.	9.5	29
47	Induction of Enzyme-like Peroxidase Activity in an Iron Porphyrin Complex Using Second Sphere Interactions. Inorganic Chemistry, 2019, 58, 2954-2964.	1.9	27
48	Synthetic Iron Porphyrins for Probing the Differences in the Electronic Structures of Heme <i>a</i>₃, Heme <i>d</i>, and Heme <i>d</i>₁. Inorganic Chemistry, 2019, 58, 152-164.	1.9	18
49	Nitrogen hybridization controls peroxo-oxo equilibrium in ethylenediamine bound binuclear [Cu2O2] complexes. Inorganica Chimica Acta, 2019, 487, 63-69.	1.2	1
50	Activation of Co(I) State in a Cobalt-Dithiolato Catalyst for Selective and Efficient CO₂ Reduction to CO. Inorganic Chemistry, 2018, 57, 5939-5947.	1.9	55
51	Functional adlayers on Au electrodes: some recent applications in hydrogen evolution and oxygen reduction. Journal of Materials Chemistry A, 2018, 6, 1323-1339.	5.2	14
52	Hydrogen Evolution from Aqueous Solutions Mediated by a Heterogenized [NiFe]â€Hydrogenase Model: Low pH Enables Catalysis through an Enzymeâ€Relevant Mechanism. Angewandte Chemie - International Edition, 2018, 57, 16001-16004.	7.2	45
53	Metal Binding to AÎ² Peptides Inhibits Interaction with Cytochrome <i>c</i>: Insights from Abiological Constructs. ACS Omega, 2018, 3, 13994-14003.	1.6	5
54	Hydrogen Evolution from Aqueous Solutions Mediated by a Heterogenized [NiFe]â€Hydrogenase Model: Low pH Enables Catalysis through an Enzymeâ€Relevant Mechanism. Angewandte Chemie, 2018, 130, 16233-16236.	1.6	9

#	ARTICLE	IF	CITATIONS
55	Oxygen-Tolerant H₂ Production by [FeFe]-H₂ase Active Site Mimics Aided by Second Sphere Proton Shuttle. Journal of the American Chemical Society, 2018, 140, 12457-12468.	6.6	58
56	Rational Design of Mononuclear Iron Porphyrins for Facile and Selective 4e^{â€“}/4H⁺ O₂ Reduction: Activation of Oâ€“O Bond by 2nd Sphere Hydrogen Bonding. Journal of the American Chemical Society, 2018, 140, 9444-9457.	6.6	99
57	Investigation of Bridgehead Effects on Reduction Potential in Alkyl and Aryl Azadithiolateâ€•Bridged (Âµâ€•SCH 2 XCH 2 S) [Fe(CO) 3] 2 Synthetic Analogues of [FeFe]â€•H 2 ase Active Site. European Journal of Inorganic Chemistry, 2018, 2018, 3633-3643.	1.0	7
58	O₂ Reduction by Biosynthetic Models of Cytochrome <i>c</i> Oxidase: Insights into Role of Proton Transfer Residues from Perturbed Active Sites Models of CcO. ACS Catalysis, 2018, 8, 8915-8924.	5.5	28
59	Activating Fe(I) Porphyrins for the Hydrogen Evolution Reaction Using Second-Sphere Proton Transfer Residues. Inorganic Chemistry, 2017, 56, 1783-1793.	1.9	81
60	Three phases in pH dependent heme abstraction from myoglobin. Journal of Inorganic Biochemistry, 2017, 172, 80-87.	1.5	7
61	Spectroscopic and Reactivity Comparisons of a Pair of bTAML Complexes with Fe^Vâ•O and Fe^{IV}â•O Units. Inorganic Chemistry, 2017, 56, 6352-6361.	1.9	51
62	Enhancing efficiency of Fe2O3 for robust and proficient solar water splitting using a highly dispersed bioinspired catalyst. Journal of Catalysis, 2017, 352, 83-92.	3.1	28
63	Development of air-stable hydrogen evolution catalysts. Chemical Communications, 2017, 53, 7707-7715.	2.2	28
64	Mechanism of Reduction of Ferric Porphyrins by Sulfide: Identification of a Low Spin Fe^{III}â€“SH Intermediate. Inorganic Chemistry, 2017, 56, 3916-3925.	1.9	17
65	Dioxygen bound cobalt corroles. Chemical Communications, 2017, 53, 877-880.	2.2	24
66	Frontiers in spectroscopic techniques in inorganic chemistry. Dalton Transactions, 2017, 46, 13163-13165.	1.6	1
67	H₂ evolution catalyzed by a FeFe-hydrogenase synthetic model covalently attached to graphite surfaces. Chemical Communications, 2017, 53, 8188-8191.	2.2	44
68	Factors Determining the Rate and Selectivity of 4e^{â€“}/4H⁺ Electrocatalytic Reduction of Dioxygen by Iron Porphyrin Complexes. Accounts of Chemical Research, 2017, 50, 1744-1753.	7.6	89
69	Molecular electrocatalysts for the oxygen reduction reaction. Nature Reviews Chemistry, 2017, 1, .	13.8	213
70	A Bifunctional Electrocatalyst for Oxygen Evolution and Oxygen Reduction Reactions in Water. Angewandte Chemie - International Edition, 2016, 55, 2350-2355.	7.2	124
71	<i>In Situ</i> Mechanistic Investigation of O₂ Reduction by Iron Porphyrin Electrocatalysts Using Surface-Enhanced Resonance Raman Spectroscopy Coupled to Rotating Disk Electrode (SERRS-RDE) Setup. ACS Catalysis, 2016, 6, 6838-6852.	5.5	45
72	Bio-inspired Electrodes. , 2016, , 89-177.		1

#	Article	IF	Citations
73	Theoretical exploration of the mechanism of formylmethanofuran dehydrogenase: the first reductive step in CO2 fixation by methanogens. Journal of Biological Inorganic Chemistry, 2016, 21, 703-713.	1.1	2
74	Iron porphyrins with a hydrogen bonding cavity: effect of weak interactions on their electronic structure and reactivity. Dalton Transactions, 2016, 45, 18796-18802.	1.6	12
75	The Way Forward in Molecular Electrocatalysis. Inorganic Chemistry, 2016, 55, 10831-10834.	1.9	11
76	Valence tautomerism in synthetic models of cytochrome P450. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 6611-6616.	3.3	33
77	Ammonium tetrathiomolybdate as a novel electrode material for convenient tuning of the kinetics of electrochemical O₂ reduction by using ironâ€“porphyrin catalysts. Journal of Materials Chemistry A, 2016, 4, 6819-6823.	5.2	13
78	Second sphere control of spin state: Differential tuning of axial ligand bonds in ferric porphyrin complexes by hydrogen bonding. Journal of Inorganic Biochemistry, 2016, 155, 82-91.	1.5	20
79	Catalytic H₂O₂ Disproportionation and Electrocatalytic O₂ Reduction by a Functional Mimic of Heme Catalase: Direct Observation of Compound 0 and Compound I in Situ. ACS Catalysis, 2016, 6, 1382-1388.	5.5	52
80	CHAPTER 9. Model Compounds for Nitric Oxide Reductase. 2-Oxoglutarate-Dependent Oxygenases, 2016, , 185-224.	0.8	0
81	Intermediates Involved in the 2e^{â€“}/2H⁺ Reduction of CO₂ to CO by Iron(0) Porphyrin. Journal of the American Chemical Society, 2015, 137, 11214-11217.	6.6	109
82	Concerted Protonâ€“Electron Transfer in Electrocatalytic O₂ Reduction by Iron Porphyrin Complexes: Axial Ligands Tuning H/D Isotope Effect. Inorganic Chemistry, 2015, 54, 2383-2392.	1.9	62
83	Effect of axial ligands on electronic structure andO₂reduction by iron porphyrin complexes: Towards a quantitative understanding of the "push effect". Journal of Porphyrins and Phthalocyanines, 2015, 19, 92-108.	0.4	35
84	Tuning the thermodynamic onset potential of electrocatalytic O₂reduction reaction by synthetic ironâ€“porphyrin complexes. Chemical Communications, 2015, 51, 10010-10013.	2.2	40
85	Electrocatalytic O₂-Reduction by Synthetic Cytochrome <i>c</i> Oxidase Mimics: Identification of a â€œBridging Peroxoâ€•Intermediate Involved in Facile 4e^{â€“}/4H⁺ O₂-Reduction. Journal of the American Chemical Society, 2015, 137, 12897-12905.	6.6	100
86	Density functional theory calculations on the active site of biotin synthase: mechanism of S transfer from the Fe2S2 cluster and the role of 1st and 2nd sphere residues. Journal of Biological Inorganic Chemistry, 2015, 20, 1147-1162.	1.1	5
87	A biosynthetic model of cytochrome c oxidase as an electrocatalyst for oxygen reduction. Nature Communications, 2015, 6, 8467.	5.8	98
88	The protonation state of thiols in self-assembled monolayers on roughened Ag/Au surfaces and nanoparticles. Physical Chemistry Chemical Physics, 2015, 17, 24866-24873.	1.3	34
89	Spectroscopic characterization of a phenolate bound Fe^{II}â€“O₂adduct: gauging the relative â€œpushâ€•effect of a phenolate axial ligand. Chemical Communications, 2014, 50, 5218-5220.	2.2	21
90	Electrocatalytic O₂reduction by a monolayer of hemin: the role of pK_aof distal and proximal oxygen of a Fe^{III}â€“OOH species in determining reactivity. Chemical Communications, 2014, 50, 12304-12307.	2.2	30

#	Article	IF	Citations
91	Heme bound amylin self-assembled monolayers on an Au electrode: an efficient bio-electrode for O2 reduction to H2O. Chemical Communications, 2014, 50, 3806.	2.2	18
92	Convenient detection of the thiol functional group using H/D isotope sensitive Raman spectroscopy. Analyst, The, 2014, 139, 2118-2121.	1.7	20
93	Resonance Raman, Electron Paramagnetic Resonance, and Density Functional Theory Calculations of a Phenolate-Bound Iron Porphyrin Complex: Electrostatic versus Covalent Contribution to Bonding. Inorganic Chemistry, 2014, 53, 7361-7370.	1.9	13
94	An acetate bound cobalt oxide catalyst for water oxidation: role of monovalent anions and cations in lowering overpotential. Physical Chemistry Chemical Physics, 2014, 16, 12221.	1.3	31
95	Self-assembly of stable oligomeric and fibrillar aggregates of Aî² peptides relevant to Alzheimer's disease: morphology dependent Cu/heme toxicity and inhibition of PROS generation. Dalton Transactions, 2014, 43, 13377.	1.6	23
96	The cobalt corrole catalyzed hydrogen evolution reaction: surprising electronic effects and characterization of key reaction intermediates. Chemical Communications, 2014, 50, 2725-2727.	2.2	134
97	Effect of Axial Ligand, Spin State, and Hydrogen Bonding on the Inner-Sphere Reorganization Energies of Functional Models of Cytochrome P450. Inorganic Chemistry, 2014, 53, 10150-10158.	1.9	21
98	Electrocatalytic O₂ Reduction by [Fe-Fe]-Hydrogenase Active Site Models. Journal of the American Chemical Society, 2014, 136, 8847-8850.	6.6	51
99	Resonance Raman and Electrocatalytic Behavior of Thiolate and Imidazole Bound Iron Porphyrin Complexes on Self Assembled Monolayers: Functional Modeling of Cytochrome P450. Inorganic Chemistry, 2013, 52, 2000-2014.	1.9	62
100	Electrocatalytic O₂ Reduction Reaction by Synthetic Analogues of Cytochrome P450 and Myoglobin: In-Situ Resonance Raman and Dynamic Electrochemistry Investigations. Inorganic Chemistry, 2013, 52, 9897-9907.	1.9	50
101	Ammonium Tetrathiomolybdate: A Versatile Catalyst for Hydrogen Evolution Reaction from Water under Ambient and Hostile Conditions. Inorganic Chemistry, 2013, 52, 14168-14177.	1.9	26
102	Tuning the apparent formal potential of covalently attached ferrocene using SAM bearing ionizable COOH groups. Electrochimica Acta, 2013, 108, 624-633.	2.6	12
103	Modular synthesis, spectroscopic characterization and in situ functionalization using â€œclickâ€• chemistry of azide terminated amide containing self-assembled monolayers. RSC Advances, 2013, 3, 17174.	1.7	11
104	Mononuclear iron hydrogenase. Coordination Chemistry Reviews, 2013, 257, 42-63.	9.5	79
105	Second Sphere Control of Redox Catalysis: Selective Reduction of O₂ to O₂^{â€“} or H₂O by an Iron Porphyrin Catalyst. Inorganic Chemistry, 2013, 52, 1443-1453.	1.9	64
106	Interaction of NO with Cu and Heme-Bound Aî² Peptides Associated with Alzheimerâ€™s Disease. Inorganic Chemistry, 2013, 52, 362-368.	1.9	14
107	Analogues of oxy-heme Aî²: reactive intermediates relevant to Alzheimer's disease. Chemical Communications, 2013, 49, 1091.	2.2	15
108	Cobalt Corrole Catalyst for Efficient Hydrogen Evolution Reaction from H₂O under Ambient Conditions: Reactivity, Spectroscopy, and Density Functional Theory Calculations. Inorganic Chemistry, 2013, 52, 3381-3387.	1.9	167

#	Article	IF	Citations
109	Electrochemical Hydrogen Production in Acidic Water by an Azadithiolate Bridged Synthetic Hydrogenese Mimic: Role of Aqueous Solvation in Lowering Overpotential. ACS Catalysis, 2013, 3, 429-436.	5.5	66
110	O2 Reduction Reaction by Biologically Relevant Anionic Ligand Bound Iron Porphyrin Complexes. Inorganic Chemistry, 2013, 52, 12963-12971.	1.9	60
111	Selective 4e^{â€“}/4H⁺ O₂ Reduction by an Iron(tetraferrocenyl)Porphyrin Complex: From Proton Transfer Followed by Electron Transfer in Organic Solvent to Proton Coupled Electron Transfer in Aqueous Medium. Inorganic Chemistry, 2013, 52, 14317-14325.	1.9	76
112	Direct observation of intermediates formed during steady-state electrocatalytic O ₂ reduction by iron porphyrins. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 8431-8436.	3.3	96
113	Photophysical and ligand binding studies of metalloporphyrins bearing hydrophilic distal superstructure. Journal of Porphyrins and Phthalocyanines, 2013, 17, 210-219.	0.4	5
114	Self-Assembled Monolayers of AÎ² peptides on Au Electrodes: An Artificial Platform for Probing the Reactivity of Redox Active Metals and Cofactors Relevant to Alzheimerâ€™s Disease. Journal of the American Chemical Society, 2012, 134, 12180-12189.	6.6	33
115	A hydrogen bond scaffold supported synthetic heme FeIIIâ€“O2âˆ’ adduct. Chemical Communications, 2012, 48, 10535.	2.2	46
116	Site-specific covalent attachment of heme proteins on self-assembled monolayers. Journal of Biological Inorganic Chemistry, 2012, 17, 1009-1023.	1.1	33
117	EPR, Resonance Raman, and DFT Calculations on Thiolate- and Imidazole-Bound Iron(III) Porphyrin Complexes: Role of the Axial Ligand in Tuning the Electronic Structure. Inorganic Chemistry, 2012, 51, 10704-10714.	1.9	47
118	Selective four electron reduction of O2 by an iron porphyrin electrocatalyst under fast and slow electron fluxes. Chemical Communications, 2012, 48, 7631.	2.2	101
119	NO and O2 reactivities of synthetic functional models of nitric oxide reductase and cytochrome c oxidase. Dalton Transactions, 2011, 40, 12633.	1.6	11
120	Density Functional Theory Calculations on the Fe₂S₂(Arg)(SCys)(SSCys)₂ Cluster in HydE: Unique Electronic Structure and Redox Properties. Inorganic Chemistry, 2011, 50, 397-399.	1.9	1
121	S K-edge XAS and DFT Calculations on SAM Dependent Pyruvate Formate-Lyase Activating Enzyme: Nature of Interaction between the Fe₄S₄ Cluster and SAM and its Role in Reactivity. Journal of the American Chemical Society, 2011, 133, 18656-18662.	6.6	45
122	S K-Edge X-Ray Absorption Spectroscopy and Density Functional Theory Studies of High and Low Spin {FeNO}⁷ Thiolate Complexes: Exchange Stabilization of Electron Delocalization in {FeNO}⁷ and {FeO₂}⁸. Inorganic Chemistry, 2011, 50, 427-436.	1.9	38
123	The Kinetics of the Interaction Between Iron(III)-Ethylenediaminetetraacetate and Peroxynitrite. Aquatic Geochemistry, 2010, 16, 483-490.	1.5	4
124	Spectroscopic Characterization and Competitive Inhibition Studies of Azide Binding to a Functional NOR Model. European Journal of Inorganic Chemistry, 2010, 2010, 4870-4874.	1.0	6
125	Density functional theory calculations on Feâ€“O and Oâ€“O cleavage of ferric hydroperoxide species: Role of axial ligand and spin state. Inorganica Chimica Acta, 2010, 363, 2762-2767.	1.2	10
126	Solvation Effects on S K-Edge XAS Spectra of Feâˆ’S Proteins: Normal and Inverse Effects on WT and Mutant Rubredoxin. Journal of the American Chemical Society, 2010, 132, 12639-12647.	6.6	22

#	ARTICLE	IF	CITATIONS
127	Density Functional Theory Calculations on the Mononuclear Non-Heme Iron Active Site of Hmd Hydrogenase: Role of the Internal Ligands in Tuning External Ligand Binding and Driving H₂ Heterolysis. Journal of the American Chemical Society, 2010, 132, 13892-13901.	6.6	49
128	Thermodynamic equilibrium between blue and green copper sites and the role of the protein in controlling function. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 4969-4974.	3.3	65
129	Role of a distal pocket in the catalytic O ₂ reduction by cytochrome <i>c</i> oxidase models immobilized on interdigitated array electrodes. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 7320-7323.	3.3	60
130	Water may inhibit oxygen binding in hemoprotein models. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 4101-4105.	3.3	37
131	O2 reduction by a functional heme/nonheme bis-iron NOR model complex. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 10528-10533.	3.3	28
132	Inhibition of Electrocatalytic O₂ Reduction of Functional CcO Models by Competitive, Non-Competitive, and Mixed Inhibitors. Inorganic Chemistry, 2009, 48, 10528-10534.	1.9	9
133	Catalytic Reduction of O₂ by Cytochrome <i>c</i> Using a Synthetic Model of Cytochrome <i>c</i> Oxidase. Journal of the American Chemical Society, 2009, 131, 5034-5035.	6.6	73
134	Spectroscopic and Computational Studies of Nitrite Reductase: Proton Induced Electron Transfer and Backbonding Contributions to Reactivity. Journal of the American Chemical Society, 2009, 131, 277-288.	6.6	95
135	Using a functional enzyme model to understand the chemistry behind hydrogen sulfide induced hibernation. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 22090-22095.	3.3	143
136	Molecular and Electronic Structure of a Nonheme Iron(II) Model Complex Containing an Ironâˆ’Carbon Bond. Inorganic Chemistry, 2009, 48, 11501-11503.	1.9	18
137	S K-edge XAS and DFT Calculations on Cytochrome P450: Covalent and Ionic Contributions to the Cysteine-Fe Bond and Their Contribution to Reactivity. Journal of the American Chemical Society, 2009, 131, 7869-7878.	6.6	64
138	Mixed valent sites in biological electron transfer. Chemical Society Reviews, 2008, 37, 623.	18.7	112
139	Interaction of nitric oxide with a functional model of cytochrome <i>c</i> oxidase. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 9892-9896.	3.3	48
140	A functional nitric oxide reductase model. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 15660-15665.	3.3	97
141	Intermediates Involved in the Two Electron Reduction of NO to N₂O by a Functional Synthetic Model of Heme Containing Bacterial NO Reductase. Journal of the American Chemical Society, 2008, 130, 16498-16499.	6.6	59
142	Model Studies of Azide Binding to Functional Analogues of CcO. Inorganic Chemistry, 2008, 47, 2916-2918.	1.9	9
143	Solvent Tuning of Electrochemical Potentials in the Active Sites of HiPIP Versus Ferredoxin. Science, 2007, 318, 1464-1468.	6.0	192
144	Sulfur K-Edge XAS and DFT Studies on NiIIComplexes with Oxidized Thiolate Ligands:Â Implications for the Roles of Oxidized Thiolates in the Active Sites of Fe and Co Nitrile Hydratase. Inorganic Chemistry, 2007, 46, 4989-4996.	1.9	34

#	Article	IF	Citations
145	Resolution of the Spectroscopy versus Crystallography Issue for NO Intermediates of Nitrite Reductase from <i>Rhodobacter </i><i>sphaeroides</i>. Journal of the American Chemical Society, 2007, 129, 10310-10311.	6.6	39
146	S K-Edge XAS and DFT Calculations on Square-Planar Ni^{II}âˆ’Thiolate Complexes:â€‰ Effects of Active and Passive H-Bonding. Inorganic Chemistry, 2007, 46, 9655-9660.	1.9	16
147	Sulfur K-Edge X-ray Absorption Spectroscopy and Density Functional Theory Calculations on Superoxide Reductase:â€‰ Role of the Axial Thiolate in Reactivity. Journal of the American Chemical Society, 2007, 129, 12418-12431.	6.6	48
148	A Functional Model for the Cysteinate-Ligated Non-Heme Iron Enzyme Superoxide Reductase (SOR). Journal of the American Chemical Society, 2006, 128, 14448-14449.	6.6	65
149	How Does Single Oxygen Atom Addition Affect the Properties of an Feâˆ’Nitrile Hydratase Analogue? The Compensatory Role of the Unmodified Thiolate. Journal of the American Chemical Society, 2006, 128, 11211-11221.	6.6	93
150	Sulfur K-Edge XAS and DFT Calculations on Nitrile Hydratase:Â Geometric and Electronic Structure of the Non-heme Iron Active Site. Journal of the American Chemical Society, 2006, 128, 533-541.	6.6	91
151	X-ray Absorption Spectroscopy and Density Functional Theory Studies of [(H3buea)FeIII-X]n-(X = S2-, O2-,) Tj ETQq1 1 0.784314 rgBT American Chemical Society, 2006, 128, 9825-9833.	6.6	42
152	Metalâ€“thiolate bonds in bioinorganic chemistry. Journal of Computational Chemistry, 2006, 27, 1415-1428.	1.5	112
153	Ligand K-edge X-ray absorption spectroscopy: covalency of ligandâ€“metal bonds. Coordination Chemistry Reviews, 2005, 249, 97-129.	9.5	326
154	Sulfur K-Edge XAS and DFT Calculations on P450 Model Complexes:â€‰ Effects of Hydrogen Bonding on Electronic Structure and Redox Potentials. Journal of the American Chemical Society, 2005, 127, 12046-12053.	6.6	82
155	Sulfur K-Edge XAS and DFT Calculations on [Fe4S4]2+Clusters:Â Effects of H-bonding and Structural Distortion on Covalency and Spin Topology. Inorganic Chemistry, 2005, 44, 8349-8354.	1.9	37
156	Ligand K-edge X-ray Absorption Spectroscopy and DFT Calculations on [Fe3S4]0,+Clusters:Â Delocalization, Redox, and Effect of the Protein Environment. Journal of the American Chemical Society, 2004, 126, 16868-16878.	6.6	35
157	Ligand K-Edge X-ray Absorption Spectroscopy of [Fe4S4]1+,2+,3+ Clusters:â€‰ Changes in Bonding and Electronic Relaxation upon Redox. Journal of the American Chemical Society, 2004, 126, 8320-8328.	6.6	43
158	Î²-Octafluorocorroles. Journal of the American Chemical Society, 2003, 125, 16300-16309.	6.6	119
159	30Ï€ Aromatic Meso-Substituted Heptaphyrin Isomers:Â Syntheses, Characterization, and Spectroscopic Studies. Journal of Organic Chemistry, 2002, 67, 6309-6319.	1.7	44
160	â€œTrueâ€•Iron(V) and Iron(VI) Porphyrins:â€‰ A First Theoretical Exploration. Journal of the American Chemical Society, 2002, 124, 3206-3207.	6.6	60
161	34Ï€ Octaphyrin:Â First Structural Characterization of a Planar, Aromatic [1.0.1.0.1.0.1.0] Octaphyrin with Inverted Heterocyclic Rings. Journal of the American Chemical Society, 2001, 123, 8620-8621.	6.6	68