Sason Shaik

List of Publications by Year
in descending order

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411 papers	37,841 citations	2669 95 h-index	4535 171 g-index
484 all docs	484 docs citations	484 times ranked	15381 citing authors

#	ARTICLE	IF	CITATIONS
1	Mechanism of Oxidation Reactions Catalyzed by Cytochrome P450 Enzymes. Chemical Reviews, 2004, 104, 3947-3980.	23.0	2,048
2	How to Conceptualize Catalytic Cycles? The Energetic Span Model. Accounts of Chemical Research, 2011, 44, 101-110.	7.6	1,372
3	Theoretical Perspective on the Structure and Mechanism of Cytochrome P450 Enzymes. Chemical Reviews, 2005, 105, 2279-2328.	23.0	1,127
4	Two-State Reactivity as a New Concept in Organometallic Chemistry. Accounts of Chemical Research, 2000, 33, 139-145.	7.6	1,099
5	P450 Enzymes: Their Structure, Reactivity, and Selectivityâ€”Modeled by QM/MM Calculations. Chemical Reviews, 2010, 110, 949-1017.	23.0	924
6	Reactivity of High-Valent Ironâ€“Oxo Species in Enzymes and Synthetic Reagents: A Tale of Many States. Accounts of Chemical Research, 2007, 40, 532-542.	7.6	507
7	A Combined Kineticâˆ’Quantum Mechanical Model for Assessment of Catalytic Cycles:Â Application to Cross-Coupling and Heck Reactions. Journal of the American Chemical Society, 2006, 128, 3355-3365.	6.6	462
8	Oriented electric fields as future smart reagents in chemistry. Nature Chemistry, 2016, 8, 1091-1098.	6.6	391
9	A Model â€œReboundâ€•Mechanism of Hydroxylation by Cytochrome P450:â€‰ Stepwise and Effectively Concerted Pathways, and Their Reactivity Patterns. Journal of the American Chemical Society, 2000, 122, 8977-8989.	6.6	385
10	Axial ligand tuning of a nonheme iron(IV)â€“oxo unit for hydrogen atom abstraction. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 19181-19186.	3.3	376
11	Valence Bond Diagrams and Chemical Reactivity. Angewandte Chemie - International Edition, 1999, 38, 586-625.	7.2	350
12	Electronic Structure Makes a Difference: Cytochrome P-450 Mediated Hydroxylations of Hydrocarbons as a Two-State Reactivity Paradigm. Chemistry - A European Journal, 1998, 4, 193-199.	1.7	346
13	Two-state reactivity mechanisms of hydroxylation and epoxidation by cytochrome P-450 revealed by theory. Current Opinion in Chemical Biology, 2002, 6, 556-567.	2.8	340
14	Two-State Reactivity in Alkane Hydroxylation by Non-Heme Ironâˆ’Oxo Complexes. Journal of the American Chemical Society, 2006, 128, 8590-8606.	6.6	331
15	A Proton-Shuttle Mechanism Mediated by the Porphyrin in Benzene Hydroxylation by Cytochrome P450 Enzymes. Journal of the American Chemical Society, 2003, 125, 7413-7424.	6.6	324
16	Two-State Reactivity in Organometallic Gas-Phase Ion Chemistry. Helvetica Chimica Acta, 1995, 78, 1393-1407.	1.0	319
17	Charge-shift bonding and its manifestations in chemistry. Nature Chemistry, 2009, 1, 443-449.	6.6	303
18	Exchange-enhanced reactivity in bond activation by metalâ€“oxo enzymes and synthetic reagents. Nature Chemistry, 2011, 3, 19-27.	6.6	300

#	ARTICLE	IF	CITATIONS
19	Searching for the Second Oxidant in the Catalytic Cycle of Cytochrome P450:Â A Theoretical Investigation of the Iron(III)-Hydroperoxo Species and Its Epoxidation Pathways. Journal of the American Chemical Society, 2002, 124, 2806-2817.	6.6	295
20	Kinetic-Quantum Chemical Model for Catalytic Cycles: The Haberâˆ’Bosch Process and the Effect of Reagent Concentration. Journal of Physical Chemistry A, 2008, 112, 6032-6041.	1.1	295
21	Structure and reactivity/selectivity control by oriented-external electric fields. Chemical Society Reviews, 2018, 47, 5125-5145.	18.7	292
22	The Elusive Oxidant Species of Cytochrome P450 Enzymes:â€‰ Characterization by Combined Quantum Mechanical/Molecular Mechanical (QM/MM) Calculations. Journal of the American Chemical Society, 2002, 124, 8142-8151.	6.6	290
23	What Factors Affect the Regioselectivity of Oxidation by Cytochrome P450? A DFT Study of Allylic Hydroxylation and Double Bond Epoxidation in a Model Reaction. Journal of the American Chemical Society, 2002, 124, 11809-11826.	6.6	289
24	Electronic Structures and Gas-Phase Reactivities of Cationic Late-Transition-Metal Oxides. Journal of the American Chemical Society, 1994, 116, 10734-10741.	6.6	285
25	Quantum Mechanical/Molecular Mechanical Investigation of the Mechanism of Câˆ’H Hydroxylation of Camphor by Cytochrome P450cam:Â Theory Supports a Two-State Rebound Mechanism. Journal of the American Chemical Society, 2004, 126, 4017-4034.	6.6	269
26	A Different Story of Ï€-DelocalizationThe Distortivity of Ï€-Electrons and Its Chemical Manifestationsâ€. Chemical Reviews, 2001, 101, 1501-1540.	23.0	267
27	External Electric Field Will Control the Selectivity of Enzymatic-Like Bond Activations. Journal of the American Chemical Society, 2004, 126, 11746-11749.	6.6	265
28	Spinâˆ’Orbit Coupling in the Oxidative Activation of Hâˆ’H by FeO+. Selection Rules and Reactivity Effects. Journal of the American Chemical Society, 1997, 119, 1773-1786.	6.6	243
29	Charge-Shift Bondingâ€”A Class of Electron-Pair Bonds That Emerges from Valence Bond Theory and Is Supported by the Electron Localization Function Approach. Chemistry - A European Journal, 2005, 11, 6358-6371.	1.7	234
30	Nature of the Feâˆ’O₂ Bonding in Oxy-Myoglobin: Effect of the Protein. Journal of the American Chemical Society, 2008, 130, 14778-14790.	6.6	234
31	Hydrogenâ€Abstraction Reactivity Patterns from Aâ€…toâ€…Y: The Valence Bond Way. Angewandte Chemie - International Edition, 2012, 51, 5556-5578.	7.2	233
32	A Valence Bond Modeling of Trends in Hydrogen Abstraction Barriers and Transition States of Hydroxylation Reactions Catalyzed by Cytochrome P450 Enzymes. Journal of the American Chemical Society, 2008, 130, 10128-10140.	6.6	232
33	On The Nature of the Halogen Bond. Journal of Chemical Theory and Computation, 2014, 10, 3726-3737.	2.3	232
34	Automatic analysis of computed catalytic cycles. Journal of Computational Chemistry, 2011, 32, 978-985.	1.5	229
35	Classical Valence Bond Approach by Modern Methods. Chemical Reviews, 2011, 111, 7557-7593.	23.0	225
36	A Predictive Pattern of Computed Barriers for Câˆ’H Hydroxylation by Compound I of Cytochrome P450. Journal of the American Chemical Society, 2004, 126, 8362-8363.	6.6	218

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37	What Makes for a Good Catalytic Cycle? A Theoretical Study of the Role of an Anionic Palladium(0) Complex in the Cross-Coupling of an Aryl Halide with an Anionic Nucleophile. Organometallics, 2005, 24, 2319-2330.	1.1	218
38	A spin-restricted ensemble-referenced Kohnâ€“Sham method and its application to diradicaloid situations. Chemical Physics Letters, 1999, 304, 429-437.	1.2	217
39	Dichotomous Hydrogen Atom Transfer vs Proton-Coupled Electron Transfer During Activation of Xâ€“H Bonds (X = C, N, O) by Nonheme Ironâ€“Oxo Complexes of Variable Basicity. Journal of the American Chemical Society, 2013, 135, 17090-17104.	6.6	216
40	The Directive of the Protein: How Does Cytochrome P450 Select the Mechanism of Dopamine Formation?. Journal of the American Chemical Society, 2011, 133, 7977-7984.	6.6	214
41	Multi-State Epoxidation of Ethene by Cytochrome P450:Â A Quantum Chemical Study. Journal of the American Chemical Society, 2001, 123, 3037-3047.	6.6	213
42	Oriented Electric Fields Accelerate Dielsâ€“Alder Reactions and Control the <i>endo</i>/<i>exo</i> Selectivity. ChemPhysChem, 2010, 11, 301-310.	1.0	208
43	A Twoâ€State Reactivity Rationale for Counterintuitive Axial Ligand Effects on the Cï£¿H Activation Reactivity of Nonheme Fe^{IV}ï£¾O Oxidants. Chemistry - A European Journal, 2008, 14, 1740-1756.	1.7	198
44	Quadruple bonding in C2 and analogous eight-valence electron species. Nature Chemistry, 2012, 4, 195-200.	6.6	198
45	Electric-Field Mediated Chemistry: Uncovering and Exploiting the Potential of (Oriented) Electric Fields to Exert Chemical Catalysis and Reaction Control. Journal of the American Chemical Society, 2020, 142, 12551-12562.	6.6	195
46	Theoretical Investigation of Câˆ’H Hydroxylation by (N4Py)FeIVO2+:Â An Oxidant More Powerful than P450?. Journal of the American Chemical Society, 2005, 127, 8026-8027.	6.6	185
47	Medium Polarization and Hydrogen Bonding Effects on Compound I of Cytochrome P450:Â What Kind of a Radical Is It Really?. Journal of the American Chemical Society, 2000, 122, 12892-12893.	6.6	171
48	A mononuclear nonheme iron(iv)-oxo complex which is more reactive than cytochrome P450 model compound I. Chemical Science, 2011, 2, 1039.	3.7	170
49	Electronic structure analysis of multistate reactivity in transition metal catalyzed reactions: the case of Câ€“H bond activation by non-heme iron(iv)â€“oxo cores. Physical Chemistry Chemical Physics, 2013, 15, 8017.	1.3	169
50	Active Species of Horseradish Peroxidase (HRP) and Cytochrome P450:Â Two Electronic Chameleons. Journal of the American Chemical Society, 2003, 125, 15779-15788.	6.6	168
51	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.	18.7	167
52	Two States and Two More in the Mechanisms of Hydroxylation and Epoxidation by Cytochrome P450. Journal of the American Chemical Society, 2005, 127, 13007-13018.	6.6	162
53	The â€œRebound Controversyâ€: An Overview and Theoretical Modeling of the Rebound Step in Câˆ’H Hydroxylation by Cytochrome P450. European Journal of Inorganic Chemistry, 2004, 2004, 207-226.	1.0	156
54	Radical Clock Substrates, Their Câˆ’H Hydroxylation Mechanism by Cytochrome P450, and Other Reactivity Patterns:Â What Does Theory Reveal about the Clocks' Behavior?. Journal of the American Chemical Society, 2004, 126, 1907-1920.	6.6	156

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55	The charge-shift bonding concept. Electron-pair bonds with very large ionic-covalent resonance energies. Journal of the American Chemical Society, 1992, 114, 7861-7866.	6.6	155
56	A Theory for Bioinorganic Chemical Reactivity of Oxometal Complexes and Analogous Oxidants: The Exchange and Orbital-Selection Rules. Accounts of Chemical Research, 2013, 46, 471-482.	7.6	154
57	Breathing-orbital valence bond method - a modern valence bond method that includes dynamic correlation. Theoretical Chemistry Accounts, 2002, 108, 255-272.	0.5	152
58	Electronic Effects on Room-Temperature, Gas-Phase Câ€“H Bond Activations by Cluster Oxides and Metal Carbides: The Methane Challenge. Journal of the American Chemical Society, 2017, 139, 17201-17212.	6.6	149
59	Theoretical Investigation of Two-State-Reactivity Pathways of Hâˆ’H Activation by FeO+:Â Additionâˆ’Elimination, â€œReboundâ€ and Oxene-Insertion Mechanisms. Journal of Physical Chemistry A, 1998, 102, 3835-3846.	1.1	145
60	A Conversation on VB vs MO Theory:â€‰ A Never-Ending Rivalry?. Accounts of Chemical Research, 2003, 36, 750-756.	7.6	144
61	The â€˜pushâ€™ effect of the thiolate ligand in cytochrome P450: a theoretical gauging. Journal of Inorganic Biochemistry, 2002, 91, 554-567.	1.5	139
62	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.	6.6	137
63	Two-State Reactivity in Low-Valent Iron-Mediated Câ€“H Activation and the Implications for Other First-Row Transition Metals. Journal of the American Chemical Society, 2016, 138, 3715-3730.	6.6	136
64	One Molecule, Two Atoms, Three Views, Four Bonds?. Angewandte Chemie - International Edition, 2013, 52, 3020-3033.	7.2	129
65	Characterization, Orbital Description, and Reactivity Patterns of Transition-Metal Oxo Species in the Gas Phase. Structure and Bonding, 2000, , 91-123.	1.0	123
66	The Valence Bond Way: Reactivity Patterns of Cytochrome P450 Enzymes and Synthetic Analogs. Accounts of Chemical Research, 2010, 43, 1154-1165.	7.6	123
67	Application of spin-restricted open-shell Kohnâ€“Sham method to atomic and molecular multiplet states. Journal of Chemical Physics, 1999, 110, 116-125.	1.2	122
68	Hydrogen Bonding Modulates the Selectivity of Enzymatic Oxidation by P450: Chameleon Oxidant Behavior by Compound I The research was supported in parts by the Israel Science Foundation (ISF), the German Israeli Binational Foundation (GIF), and by the Ministry of Science, Culture, and Sports. F.O. thanks the European community for a Marie Curie Fellowship.. Angewandte Chemie - International Edition, 2002, 41, 1947.	7.2	122
69	Can a Single Oxidant with Two Spin States Masquerade as Two Different Oxidants? A Study of the Sulfoxidation Mechanism by Cytochrome P450. Journal of the American Chemical Society, 2003, 125, 8698-8699.	6.6	120
70	The Inverted Bond in [1.1.1]Propellane is a Chargeâ€Shift Bond. Angewandte Chemie - International Edition, 2009, 48, 1407-1410.	7.2	120
71	The Fundamental Role of Exchangeâ€Enhanced Reactivity in Cï£¿H Activation by <i>S</i>=2 Oxo Iron(IV) Complexes. Angewandte Chemie - International Edition, 2010, 49, 3342-3345.	7.2	117
72	QM/MM Studies into the H₂O₂-Dependent Activity of Lytic Polysaccharide Monooxygenases: Evidence for the Formation of a Caged Hydroxyl Radical Intermediate. ACS Catalysis, 2018, 8, 1346-1351.	5.5	117

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73	Exchange-Enhanced H-Abstraction Reactivity of High-Valent Nonheme Iron(IV)-Oxo from Coupled Cluster and Density Functional Theories. Journal of Physical Chemistry Letters, 2010, 1, 1533-1540.	2.1	116
74	Cytochrome P450â€”The Wonderful Nanomachine Revealed through Dynamic Simulations of the Catalytic Cycle. Accounts of Chemical Research, 2019, 52, 389-399.	7.6	116
75	What is the Active Species of Cytochrome P450 during Camphor Hydroxylation? QM/MM Studies of Different Electronic States of Compound I and of Reduced and Oxidized Ironâˆ’Oxo Intermediates. Journal of the American Chemical Society, 2007, 129, 8978-8987.	6.6	115
76	Chameleon States: High-Valent Metal-Oxo Species of Cytochrome P450 and Its Ruthenium Analogue. Angewandte Chemie - International Edition, 2001, 40, 2874-2878.	7.2	114
77	Theoretical Study of N-Demethylation of Substituted N,N-Dimethylanilines by Cytochrome P450:â€‰ The Mechanistic Significance of Kinetic Isotope Effect Profiles. Journal of Physical Chemistry B, 2007, 111, 7700-7710.	1.2	113
78	Assessment of Theoretical Methods for Complexes of Gold(I) and Gold(III) with Unsaturated Aliphatic Hydrocarbon: Which Density Functional Should We Choose?. Journal of Chemical Theory and Computation, 2011, 7, 4002-4011.	2.3	113
79	Oriented-External Electric Fields Create Absolute Enantioselectivity in Dielsâ€“Alder Reactions: Importance of the Molecular Dipole Moment. Journal of the American Chemical Society, 2018, 140, 13350-13359.	6.6	113
80	Understanding the Nature of the CHÂ·Â·Â·HC Interactions in Alkanes. Journal of Chemical Theory and Computation, 2013, 9, 1977-1991.	2.3	112
81	A Twoâ€State Reactivity Model Explains Unusual Kinetic Isotope Effect Patterns in Cï£¿H Bond Cleavage by Nonheme Oxoiron(IV) Complexes. Angewandte Chemie - International Edition, 2009, 48, 1291-1295.	7.2	111
82	Enhanced Reactivities of Iron(IV)â€Oxo Porphyrin Ï€â€Cation Radicals in Oxygenation Reactions by Electronâ€Donating Axial Ligands. Chemistry - A European Journal, 2009, 15, 10039-10046.	1.7	110
83	Reactivity patterns of cytochrome P450 enzymes: multifunctionality of the active species, and the two statesâ€“two oxidants conundrum. Natural Product Reports, 2007, 24, 533-552.	5.2	109
84	Multistate Reactivity in Styrene Epoxidation by Compound I of Cytochrome P450: Mechanisms of Products and Side Products Formation. Chemistry - A European Journal, 2005, 11, 2825-2835.	1.7	108
85	Active Anionic Zero-Valent Palladium Catalysts: Characterization by Density Functional Calculations. Chemistry - A European Journal, 2004, 10, 3072-3080.	1.7	107
86	QM/MM Study of Mechanisms for Compound I Formation in the Catalytic Cycle of Cytochrome P450cam. Journal of the American Chemical Society, 2006, 128, 13204-13215.	6.6	105
87	The Effect of Heme Environment on the Hydrogen Abstraction Reaction of Camphor in P450camCatalysis:Â A QM/MM Study. Journal of the American Chemical Society, 2006, 128, 3924-3925.	6.6	105
88	Theoretical Characterization of Substrate Access/Exit Channels in the Human Cytochrome P450 3A4 Enzyme: Involvement of Phenylalanine Residues in the Gating Mechanism. Journal of Physical Chemistry B, 2009, 113, 13018-13025.	1.2	105
89	External electric field effects on chemical structure and reactivity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1438.	6.2	104
90	The Poulosâˆ’Kraut Mechanism of Compound I Formation in Horseradish Peroxidase:Â A QM/MM Study. Journal of Physical Chemistry B, 2006, 110, 10526-10533.	1.2	101

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91	Structure and quantum chemical characterization of chloroperoxidase compound 0, a common reaction intermediate of diverse heme enzymes. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 99-104.	3.3	100
92	The Effect of a Water Molecule on the Mechanism of Formation of Compound 0 in Horseradish Peroxidase. Journal of the American Chemical Society, 2007, 129, 6346-6347.	6.6	99
93	Computation Sheds Insight into Iron Porphyrin Carbenesâ€™ Electronic Structure, Formation, and Nâ€“H Insertion Reactivity. Journal of the American Chemical Society, 2016, 138, 9597-9610.	6.6	99
94	Chemistry is about energy and its changes: A critique of bond-length/bond-strength correlations. Coordination Chemistry Reviews, 2017, 344, 355-362.	9.5	99
95	Two-State Reactivity in the Rebound Step of Alkane Hydroxylation by Cytochrome P-450: Origins of Free Radicals with Finite Lifetimes. Angewandte Chemie - International Edition, 2000, 39, 2003-2007.	7.2	98
96	Topology of Electron Charge Density for Chemical Bonds from Valence Bond Theory: A Probe of Bonding Types. Chemistry - A European Journal, 2009, 15, 2979-2989.	1.7	98
97	Is the avoided crossing state a good approximation for the transition state of a chemical reaction? An analysis of Menschutkin and ionic SN2 reactions. Journal of the American Chemical Society, 1994, 116, 262-273.	6.6	97
98	The High-Valent Compound of Cytochrome P450: The Nature of the Feâˆ’S Bond and the Role of the Thiolate Ligand as an Internal Electron Donor. Angewandte Chemie - International Edition, 2000, 39, 3851-3855.	7.2	97
99	Effect of External Electric Fields on the Câˆ’H Bond Activation Reactivity of Nonheme Ironâˆ’Oxo Reagents. Journal of the American Chemical Society, 2008, 130, 3319-3327.	6.6	97
100	Electrostatic and Charge-Induced Methane Activation by a Concerted Double Câ€“H Bond Insertion. Journal of the American Chemical Society, 2017, 139, 1684-1689.	6.6	96
101	Electrophilic Aromatic Chlorination and Haloperoxidation of Chloride Catalyzed by Polyfluorinated Alcohols:Â A New Manifestation of Template Catalysis. Journal of the American Chemical Society, 2003, 125, 12116-12117.	6.6	94
102	How Does Product Isotope Effect Prove the Operation of a Two-State â€œReboundâ€•Mechanism in Câˆ’H Hydroxylation by Cytochrome P450?. Journal of the American Chemical Society, 2003, 125, 13024-13025.	6.6	93
103	Characterization of Manganese(V)âˆ’Oxo Polyoxometalate Intermediates and Their Properties in Oxygen-Transfer Reactions. Journal of the American Chemical Society, 2006, 128, 15451-15460.	6.6	92
104	Origins of the Exalted b2uFrequency in the First Excited State of Benzene. Journal of the American Chemical Society, 1996, 118, 666-671.	6.6	91
105	The High-Valent Ironâˆ’Oxo Species of Polyoxometalate, if It Can Be Made, Will Be a Highly Potent Catalyst for Câˆ’H Hydroxylation and Double-Bond Epoxidation. Journal of the American Chemical Society, 2005, 127, 17712-17718.	6.6	90
106	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.	7.2	90
107	Electronic Origins of the Variable Efficiency of Room-Temperature Methane Activation by Homo- and Heteronuclear Cluster Oxide Cations [XYO₂]⁺ (X, Y = Al, Si, Mg): Competition between Proton-Coupled Electron Transfer and Hydrogen-Atom Transfer. Journal of the American Chemical Society, 2016, 138, 7973-7981.	6.6	90
108	How Does Ethene Inactivate Cytochrome P450 En Route to Its Epoxidation? A Density Functional Study. Angewandte Chemie - International Edition, 2001, 40, 2871-2874.	7.2	89

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109	Structural Characterization of the Fleeting Ferric Peroxo Species in Myoglobin:â€‰ Experiment and Theory. Journal of the American Chemical Society, 2007, 129, 13394-13395.	6.6	89
110	On the Role of Water in Peroxidase Catalysis: A Theoretical Investigation of HRP Compound I Formation. Journal of Physical Chemistry B, 2010, 114, 5161-5169.	1.2	89
111	How Does Tunneling Contribute to Counterintuitive H-Abstraction Reactivity of Nonheme Fe(IV)O Oxidants with Alkanes?. Journal of the American Chemical Society, 2015, 137, 722-733.	6.6	89
112	What Is the Difference between the Manganese Porphyrin and Corrole Analogues of Cytochrome P450's Compound I?. Chemistry - A European Journal, 2001, 7, 4954-4960.	1.7	88
113	A KekulÃ©-Crossing Model for the â€œAnomalousâ€•Behavior of the b2u Modes of Aromatic Hydrocarbons in the Lowest Excited 1B2u State. Accounts of Chemical Research, 1996, 29, 211-218.	7.6	86
114	On the â€œReboundâ€•Mechanism of Alkane Hydroxylation by Cytochrome P450: Electronic Structure of the Intermediate and the Electron Transfer Character in the Rebound Step. Angewandte Chemie - International Edition, 1999, 38, 3510-3512.	7.2	86
115	One oxidant, many pathways: a theoretical perspective of monooxygenation mechanisms by cytochrome P450 enzymes. Journal of Biological Inorganic Chemistry, 2004, 9, 661-668.	1.1	86
116	Identification of a low-spin acylperoxoiron(III) intermediate in bio-inspired non-heme iron-catalysed oxidations. Nature Communications, 2014, 5, 3046.	5.8	86
117	The Experimentally Elusive Oxidant of Cytochrome P450: A Theoretical â€œTrappingâ€•Defining More Closely the â€œRealâ€•Species. ChemBioChem, 2001, 2, 848.	1.3	85
118	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.	6.6	85
119	Mechanistic Variants in Gas-Phase Metal-Oxide Mediated Activation of Methane at Ambient Conditions. Journal of the American Chemical Society, 2016, 138, 11368-11377.	6.6	85
120	Molecular Dynamics and QM/MM Calculations Predict the Substrate-Induced Gating of Cytochrome P450 BM3 and the Regio- and Stereoselectivity of Fatty Acid Hydroxylation. Journal of the American Chemical Society, 2016, 138, 837-845.	6.6	85
121	Systematic QM/MM investigation of factors that affect the cytochrome P450-catalyzed hydrogen abstraction of camphor. Journal of Computational Chemistry, 2006, 27, 1324-1337.	1.5	84
122	Chargeâ€•Shift Bonding: A New and Unique Form of Bonding. Angewandte Chemie - International Edition, 2020, 59, 984-1001.	7.2	84
123	Kinetic Isotope Effect is a Sensitive Probe of Spin State Reactivity in Câˆ’H Hydroxylation ofN,N-Dimethylaniline by Cytochrome P450. Journal of the American Chemical Society, 2006, 128, 394-395.	6.6	82
124	A survey of recent developments in ab initio valence bond theory. Journal of Computational Chemistry, 2007, 28, 137-151.	1.5	82
125	Multireference and Multiconfiguration Ab Initio Methods in Heme-Related Systems: What Have We Learned So Far?. Journal of Physical Chemistry B, 2011, 115, 1727-1742.	1.2	82
126	Valence Bond Mixing and Curve Crossing Diagrams in Chemical Reactivity and Bonding. Advances in Quantum Chemistry, 1995, , 99-163.	0.4	80

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127	Valence Bond Configuration Interaction:â€‰ A Practical ab Initio Valence Bond Method That Incorporates Dynamic Correlation. Journal of Physical Chemistry A, 2002, 106, 2721-2726.	1.1	79
128	Oxygen Economy of Cytochrome P450:Â What Is the Origin of the Mixed Functionality as a Dehydrogenaseâˆ'Oxidase Enzyme Compared with Its Normal Function?. Journal of the American Chemical Society, 2004, 126, 5072-5073.	6.6	78
129	Why Is Cobalt the Best Transition Metal in Transition-Metal Hangman Corroles for Oâ€"O Bond Formation during Water Oxidation?. Journal of Physical Chemistry Letters, 2012, 3, 2315-2319.	2.1	78
130	Principal Active Species of Horseradish Peroxidase, Compound I:Â A Hybrid Quantum Mechanical/Molecular Mechanical Study. Journal of the American Chemical Society, 2005, 127, 13611-13621.	6.6	77
131	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.	2.1	77
132	The Nature of the Fourth Bond in the Ground State of C₂: The Quadruple Bond Conundrum. Chemistry - A European Journal, 2014, 20, 6220-6232.	1.7	77
133	A Single Transition State Serves Two Mechanisms:ÂAn ab Initio Classical Trajectory Study of the Electron Transfer and Substitution Mechanisms in Reactions of Ketyl Radical Anions with Alkyl Halides. Journal of the American Chemical Society, 2001, 123, 130-134.	6.6	76
134	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.	2.1	76
135	Interplay of Tunneling, Two-State Reactivity, and Bellâ€"Evansâ€"Polanyi Effects in Câ€"H Activation by Nonheme Fe(IV)O Oxidants. Journal of the American Chemical Society, 2016, 138, 2094-2097.	6.6	76
136	Bonding Conundrums in the C₂ Molecule: A Valence Bond Study. Journal of Chemical Theory and Computation, 2011, 7, 121-130.	2.3	75
137	Kinetic Isotope Effect Determination Probes the Spin of the Transition State, Its Stereochemistry, and Its Ligand Sphere in Hydrogen Abstraction Reactions of Oxoiron(IV) Complexes. Accounts of Chemical Research, 2018, 51, 107-117.	7.6	75
138	Is the Ruthenium Analogue of Compound I of Cytochrome P450 an Efficient Oxidant? A Theoretical Investigation of the Methane Hydroxylation Reaction. Journal of the American Chemical Society, 2003, 125, 2291-2300.	6.6	74
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