

Kazunari Yoshizawa

List of Publications by Year in descending order

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331
papers

13,148
citations

17429

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36008

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docs citations

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times ranked

10229
citing authors

#	ARTICLE	IF	CITATIONS
1	Computational Prediction for Singlet- and Triplet-Transition Energies of Charge-Transfer Compounds. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3872-3877.	2.3	312
2	Methane-to-Methanol Conversion by First-Row Transition-Metal Oxide Ions: ScO^+ , TiO^+ , VO^+ , CrO^+ , MnO^+ , FeO^+ , CoO^+ , NiO^+ , and CuO^+ . <i>Journal of the American Chemical Society</i> , 2000, 122, 12317-12326.	6.6	262
3	Catalytic transformation of dinitrogen into ammonia and hydrazine by iron-dinitrogen complexes bearing pincer ligand. <i>Nature Communications</i> , 2016, 7, 12181.	5.8	244
4	Orbital Views of the Electron Transport in Molecular Devices. <i>Journal of the American Chemical Society</i> , 2008, 130, 9406-9413.	6.6	223
5	Catalytic Reduction of Dinitrogen to Ammonia by Use of Molybdenum Nitride Complexes Bearing a Tridentate Triphosphine as Catalysts. <i>Journal of the American Chemical Society</i> , 2015, 137, 5666-5669.	6.6	215
6	Catalytic Formation of Ammonia from Molecular Dinitrogen by Use of Dinitrogen-Bridged Dimolybdenum Dinitrogen Complexes Bearing PNP-Pincer Ligands: Remarkable Effect of Substituent at PNP-Pincer Ligand. <i>Journal of the American Chemical Society</i> , 2014, 136, 9719-9731.	6.6	202
7	Interplay between Theory and Experiment for Ammonia Synthesis Catalyzed by Transition Metal Complexes. <i>Accounts of Chemical Research</i> , 2016, 49, 987-995.	7.6	200
8	Remarkable catalytic activity of dinitrogen-bridged dimolybdenum complexes bearing NHC-based PCP-pincer ligands toward nitrogen fixation. <i>Nature Communications</i> , 2017, 8, 14874.	5.8	198
9	Intrinsic reaction coordinate analysis of the conversion of methane to methanol by an iron oxo species: A study of crossing seams of potential energy surfaces. <i>Journal of Chemical Physics</i> , 1999, 111, 538-545.	1.2	191
10	Direct Transformation of Molecular Dinitrogen into Ammonia Catalyzed by Cobalt Dinitrogen Complexes Bearing Anionic PNP Pincer Ligands. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 14291-14295.	7.2	184
11	Methane to Methanol Conversion by MnO^+ , FeO^+ , and CoO^+ : A Theoretical Study of Catalytic Selectivity. <i>Journal of the American Chemical Society</i> , 1998, 120, 564-572.	6.6	164
12	A light-induced spin crossover actuated single-chain magnet. <i>Nature Communications</i> , 2013, 4, .	5.8	162
13	Unique behaviour of dinitrogen-bridged dimolybdenum complexes bearing pincer ligand towards catalytic formation of ammonia. <i>Nature Communications</i> , 2014, 5, 3737.	5.8	162
14	Catalytic Nitrogen Fixation via Direct Cleavage of Nitrogen Nitrogen Triple Bond of Molecular Dinitrogen under Ambient Reaction Conditions. <i>Bulletin of the Chemical Society of Japan</i> , 2017, 90, 1111-1118.	2.0	156
15	Molybdenum-Catalyzed Transformation of Molecular Dinitrogen into Silylamine: Experimental and DFT Study on the Remarkable Role of Ferrocenyldiphosphine Ligands. <i>Journal of the American Chemical Society</i> , 2011, 133, 3498-3506.	6.6	148
16	Methane selective oxidation to methanol by metal-exchanged zeolites: a review of active sites and their reactivity. <i>Catalysis Science and Technology</i> , 2019, 9, 1744-1768.	2.1	148
17	Conversion of Methane to Methanol at the Mononuclear and Dinuclear Copper Sites of Particulate Methane Monooxygenase (pMMO): A DFT and QM/MM Study. <i>Journal of the American Chemical Society</i> , 2006, 128, 9873-9881.	6.6	146
18	Direct Conversion of Methane to Methanol by Metal-Exchanged ZSM-5 Zeolite (Metal = Fe, Co, Ni, Cu). <i>ACS Catalysis</i> , 2016, 6, 8321-8331.	5.5	141

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19	Direct Methane to Methanol and Benzene to Phenol Conversions on Fe-ZSM-5 Zeolite: Theoretical Predictions on the Reaction Pathways and Energetics. <i>Journal of Physical Chemistry B</i> , 2000, 104, 734-740.	1.2	139
20	Sulfur-Gold Orbital Interactions which Determine the Structure of Alkanethiolate/Au(111) Self-Assembled Monolayer Systems. <i>Journal of Physical Chemistry B</i> , 2002, 106, 12727-12736.	1.2	135
21	An Orbital Rule for Electron Transport in Molecules. <i>Accounts of Chemical Research</i> , 2012, 45, 1612-1621.	7.6	135
22	Ruthenium-Catalyzed Selective and Efficient Oxygenation of Hydrocarbons with Water as an Oxygen Source. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 5772-5776.	7.2	133
23	Roles of Zeolite Confinement and Cu-Cu Angle on the Direct Conversion of Methane to Methanol by [Cu ₂ ($\frac{1}{4}$ -O)] ²⁺ -Exchanged AEI, CHA, AFX, and MFI Zeolites. <i>ACS Catalysis</i> , 2017, 7, 3741-3751.	5.5	129
24	Molecular Understanding of the Adhesive Force between a Metal Oxide Surface and an Epoxy Resin. <i>Journal of Physical Chemistry C</i> , 2011, 115, 11701-11708.	1.5	126
25	Catalytic Mechanism of Dopamine \hat{I}^2 -Monooxygenase Mediated by Cu(III)-Oxo. <i>Inorganic Chemistry</i> , 2006, 45, 3034-3041.	1.9	123
26	Theoretical Study of Donor- \hat{I} -Bridge-Acceptor Unimolecular Electric Rectifier. <i>Journal of Physical Chemistry C</i> , 2007, 111, 11699-11705.	1.5	121
27	Theoretical Study of the Direct Synthesis of H ₂ O ₂ on Pd and Pd/Au Surfaces. <i>Journal of Physical Chemistry C</i> , 2008, 112, 19501-19505.	1.5	121
28	Abstraction of the Hydrogen Atom of Methane by Iron-Oxo Species: The Concerted Reaction Path Is Energetically More Favorable. <i>Organometallics</i> , 1998, 17, 2825-2831.	1.1	119
29	Iron-catalysed transformation of molecular dinitrogen into silylamine under ambient conditions. <i>Nature Communications</i> , 2012, 3, 1254.	5.8	118
30	Reaction Paths for the Conversion of Methane to Methanol Catalyzed by FeO ⁺ . <i>Chemistry - A European Journal</i> , 1997, 3, 1160-1169.	1.7	114
31	Nonradical Mechanism for Methane Hydroxylation by Iron-Oxo Complexes. <i>Accounts of Chemical Research</i> , 2006, 39, 375-382.	7.6	111
32	Cleavage and Formation of Molecular Dinitrogen in a Single System Assisted by Molybdenum Complexes Bearing Ferrocenyldiphosphine. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 11488-11492.	7.2	111
33	Molecular motor-driven abrupt anisotropic shape change in a single crystal of a Ni complex. <i>Nature Chemistry</i> , 2014, 6, 1079-1083.	6.6	111
34	Catalytic Reduction of Molecular Dinitrogen to Ammonia and Hydrazine Using Vanadium Complexes. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 9064-9068.	7.2	109
35	The role of orbital interactions in determining ferromagnetic coupling in organic molecular assemblies. <i>Journal of the American Chemical Society</i> , 1995, 117, 6921-6926.	6.6	107
36	A ferromagnetically coupled Fe ₄₂ cyanide-bridged nanocage. <i>Nature Communications</i> , 2015, 6, 5955.	5.8	104

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37	Methane Partial Oxidation over $[\text{Cu}^{2+}(\text{O})^{1/4}]^{2+}$ and $[\text{Cu}^{3+}(\text{O})^{3/4}]^{3+}$ Active Species in Large-Pore Zeolites. ACS Catalysis, 2018, 8, 1500-1509.	5.5	104
38	Comparison of the Reactivity of $\text{Bis}(\text{O})\text{Cu}^{\text{II}}\text{Cu}^{\text{III}}$ and $\text{Cu}^{\text{III}}\text{Cu}^{\text{III}}$ Species to Methane. Inorganic Chemistry, 2009, 48, 838-845.	1.9	102
39	Nitrogen fixation catalyzed by ferrocene-substituted dinitrogen-bridged dimolybdenum dinitrogen complexes: unique behavior of ferrocene moiety as redox active site. Chemical Science, 2015, 6, 3940-3951.	3.7	100
40	Dioxygen Cleavage and Methane Activation on Diiron Enzyme Models: A Theoretical Study. Journal of the American Chemical Society, 1997, 119, 12311-12321.	6.6	97
41	A spin-orbit coupling study on the spin inversion processes in the direct methane-to-methanol conversion by FeO^+ . Journal of Chemical Physics, 2003, 118, 5872-5879.	1.2	97
42	Orbital Views of Molecular Conductance Perturbed by Anchor Units. Journal of the American Chemical Society, 2011, 133, 5955-5965.	6.6	94
43	Reaction Pathway for the Direct Benzene Hydroxylation by Iron Oxo Species. Journal of the American Chemical Society, 1999, 121, 147-153.	6.6	91
44	Quantum Transport Effects in Nanosized Graphite Sheets. ChemPhysChem, 2002, 3, 1035-1037.	1.0	90
45	Theoretical Study of the Decomposition and Hydrogenation of H_2O_2 on Pd and Au@Pd Surfaces: Understanding toward High Selectivity of H_2O_2 Synthesis. Journal of Physical Chemistry C, 2011, 115, 7392-7398.	1.5	90
46	Dependence of Single-Molecule Conductance on Molecule Junction Symmetry. Journal of the American Chemical Society, 2011, 133, 11426-11429.	6.6	89
47	Theoretical Revisit of the Direct Synthesis of H_2O_2 on Pd and Au@Pd Surfaces: A Comprehensive Mechanistic Study. Journal of Physical Chemistry C, 2011, 115, 25359-25367.	1.5	89
48	Theoretical Overview of Methane Hydroxylation by Copper Oxo Species in Enzymatic and Zeolitic Catalysts. Accounts of Chemical Research, 2018, 51, 2382-2390.	7.6	85
49	Adsorption and Activation of Methane on the (110) Surface of Rutile-type Metal Dioxides. Journal of Physical Chemistry C, 2018, 122, 15359-15381.	1.5	85
50	Computational Exploration of the Catalytic Mechanism of Dopamine O_2 -Monooxygenase: Modeling of Its Mononuclear Copper Active Sites. Inorganic Chemistry, 2005, 44, 4226-4236.	1.9	82
51	Photoswitching of Conductivity through a Diarylperfluorocyclopentene Nanowire. Journal of Physical Chemistry C, 2007, 111, 3517-3521.	1.5	82
52	Cobalt-Catalyzed Transformation of Molecular Dinitrogen into Silylamine under Ambient Reaction Conditions. Chemistry - A European Journal, 2015, 21, 8905-8909.	1.7	80
53	Specific Enhancement of Catalytic Activity by a Dicopper Core: Selective Hydroxylation of Benzene to Phenol with Hydrogen Peroxide. Angewandte Chemie - International Edition, 2017, 56, 7779-7782.	7.2	77
54	A Low-Spin Ruthenium(IV) Oxo Complex: Does the Spin State Have an Impact on the Reactivity?. Angewandte Chemie - International Edition, 2010, 49, 8449-8453.	7.2	76

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55	Mechanistic Study on the Production of Hydrogen Peroxide in the Anthraquinone Process. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 4113-4120.	1.2	76
56	Theoretical Study of Long-Range Electron Transport in Molecular Junctions. <i>Journal of Physical Chemistry C</i> , 2008, 112, 17408-17415.	1.5	73
57	Homogeneous Photocatalytic Water Oxidation with a Dinuclear Co ^{III} -Pyridylmethylamine Complex. <i>Inorganic Chemistry</i> , 2016, 55, 1154-1164.	1.9	73
58	Electron-phonon coupling in negatively charged acene- and phenanthrene-edge-type hydrocarbon crystals. <i>Journal of Chemical Physics</i> , 2002, 116, 3420-3429.	1.2	72
59	Quantum Chemical Approach to the Mechanism for the Biological Conversion of Tyrosine to Dopaquinone. <i>Journal of the American Chemical Society</i> , 2008, 130, 16890-16897.	6.6	70
60	Two-step concerted mechanism for alkane hydroxylation on the ferryl active site of methane monooxygenase. <i>Journal of Biological Inorganic Chemistry</i> , 1998, 3, 318-324.	1.1	69
61	Assembling an alkyl rotor to access abrupt and reversible crystalline deformation of a cobalt(II) complex. <i>Nature Communications</i> , 2015, 6, 8810.	5.8	69
62	Wire-Length Dependence of the Conductance of Oligo(p-phenylene) Dithiolate Wires: A Consideration from Molecular Orbitals. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9143-9149.	1.1	66
63	Bistability of Magnetization without Spin-Transition in a High-Spin Cobalt(II) Complex due to Angular Momentum Quenching. <i>Journal of the American Chemical Society</i> , 2009, 131, 4560-4561.	6.6	63
64	Role of Edge Oxygen Atoms on the Adhesive Interaction between Carbon Fiber and Epoxy Resin. <i>Journal of Physical Chemistry C</i> , 2013, 117, 24830-24835.	1.5	60
65	Role of Tyrosine Residue in Methane Activation at the Dicopper Site of Particulate Methane Monooxygenase: A Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2013, 52, 7907-7917.	1.9	58
66	Superior thermoelasticity and shape-memory nanopores in a porous supramolecular organic framework. <i>Nature Communications</i> , 2016, 7, 11564.	5.8	58
67	Molecular Understanding of the Adhesive Force between a Metal Oxide Surface and an Epoxy Resin: Effects of Surface Water. <i>Bulletin of the Chemical Society of Japan</i> , 2012, 85, 672-678.	2.0	57
68	Dioxygen Binding to Dinuclear Iron Centers on Methane Monooxygenase Models. <i>Inorganic Chemistry</i> , 1996, 35, 2409-2410.	1.9	56
69	Formation of an Iron-Oxo Species upon Decomposition of Dinitrogen Oxide on a Model of Fe-ZSM-5 Zeolite. <i>Bulletin of the Chemical Society of Japan</i> , 2000, 73, 29-36.	2.0	56
70	A Theoretical Study of Alcohol Oxidation by Ferrate. <i>Journal of Organic Chemistry</i> , 2001, 66, 4122-4131.	1.7	56
71	Surface Oxygen Atom as a Cooperative Ligand in Pd Nanoparticle Catalysis for Selective Hydration of Nitriles to Amides in Water: Experimental and Theoretical Studies. <i>ACS Catalysis</i> , 2012, 2, 2467-2474.	5.5	56
72	Multiply-fused porphyrins effects of extended π -conjugation on the optical and electrochemical properties. <i>Chemical Communications</i> , 2013, 49, 5939.	2.2	56

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73	Direct Transformation of Molecular Dinitrogen into Ammonia Catalyzed by Cobalt Dinitrogen Complexes Bearing Anionic PNP Pincer Ligands. <i>Angewandte Chemie</i> , 2016, 128, 14503-14507.	1.6	56
74	Greenâ€™s function formalism coupled with Gaussian broadening of discrete states for quantum transport: Application to atomic and molecular wires. <i>Journal of Chemical Physics</i> , 2004, 121, 8050.	1.2	55
75	Conversion of Methane to Methanol on Diiron and Dicopper Enzyme Models of Methane Monooxygenase: A Theoretical Study on a Concerted Reaction Pathway. <i>Bulletin of the Chemical Society of Japan</i> , 2000, 73, 815-827.	2.0	54
76	Potential Linearâ€™Chain Organic Ferromagnets. <i>Chemistry - A European Journal</i> , 1995, 1, 403-413.	1.7	53
77	Reaction Pathways for the Oxidation of Methanol to Formaldehyde by an Ironâ€™Oxo Species. <i>Journal of Physical Chemistry A</i> , 2000, 104, 9347-9355.	1.1	50
78	Orbital Control of the Conductance Photoswitching in Diarylethene. <i>Journal of Physical Chemistry C</i> , 2009, 113, 21477-21483.	1.5	50
79	Kinetic Isotope Effects in a Câ€™H Bond Dissociation by the Iron-Oxo Species of Cytochrome P450. <i>Journal of Physical Chemistry B</i> , 2000, 104, 12365-12370.	1.2	49
80	DFT Study on Chemical N ₂ Fixation by Using a Cubane-Type Ru ₃ S ₄ Cluster: Energy Profile for Binding and Reduction of N ₂ to Ammonia via Ruâ€™Nâ€™NH _x (<i>x</i> = 1â€™3) Intermediates with Unique Structures. <i>Journal of the American Chemical Society</i> , 2008, 130, 9037-9047.	6.6	49
81	Photochemical Reversibility of Ring-Closing and Ring-Opening Reactions in Diarylperfluorocyclopentenes. <i>Journal of Physical Chemistry C</i> , 2009, 113, 3826-3834.	1.5	48
82	Molybdenum-Catalyzed Ammonia Formation Using Simple Monodentate and Bidentate Phosphines as Auxiliary Ligands. <i>Inorganic Chemistry</i> , 2019, 58, 8927-8932.	1.9	48
83	Methane Activation at the Metalâ€™Support Interface of Ni ₄ â€™CeO ₂ (111) Catalyst: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 9788-9798.	1.5	48
84	Mechanistic Insights into Homogeneous Electrocatalytic and Photocatalytic Hydrogen Evolution Catalyzed by High-Spin Ni(II) Complexes with S ₂ N ₂ -Type Tetradentate Ligands. <i>Inorganic Chemistry</i> , 2018, 57, 7180-7190.	1.9	47
85	Methane Hydroxylation on a Diiron Model of Soluble Methane Monooxygenase. <i>Bulletin of the Chemical Society of Japan</i> , 1998, 71, 1899-1909.	2.0	46
86	Directional Electron Transfer in Crystals of [CrCo] Dinuclear Complexes Achieved by Chirality-Assisted Preparative Method. <i>Journal of the American Chemical Society</i> , 2016, 138, 14170-14173.	6.6	46
87	An Azuleneâ€™Fused Tetracene Diimide with a Small HOMOâ€™LUMO Gap. <i>ChemPlusChem</i> , 2017, 82, 1010-1014.	1.3	45
88	Ground-State Copper(III) Stabilized by N-Confused/N-Linked Corroles: Synthesis, Characterization, and Redox Reactivity. <i>Journal of the American Chemical Society</i> , 2018, 140, 6883-6892.	6.6	45
89	Molecular understanding of the adhesive interactions between silica surface and epoxy resin: Effects of interfacial water. <i>Journal of Computational Chemistry</i> , 2019, 40, 164-171.	1.5	45
90	Adhesion of Epoxy Resin with Hexagonal Boron Nitride and Graphite. <i>ACS Omega</i> , 2019, 4, 4491-4504.	1.6	43

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91	Analysis of Photoinduced Magnetization in a (Co, Fe) Prussian Blue Model. <i>Journal of Physical Chemistry B</i> , 1998, 102, 5432-5437.	1.2	42
92	Macroscopic Polarization Change via Electron Transfer in a Valence Tautomeric Cobalt Complex. <i>Nature Communications</i> , 2020, 11, 1992.	5.8	41
93	Plasma polymerization of 1-benzothiophene. <i>Journal of Applied Physics</i> , 1991, 70, 5653-5660.	1.1	40
94	Femtosecond Dynamics of the Methane \rightarrow Methanol and Benzene \rightarrow Phenol Conversions by an Iron \rightarrow Oxo Species. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2552-2561.	1.1	40
95	Conductance through Short DNA Molecules. <i>Journal of Physical Chemistry C</i> , 2011, 115, 3481-3490.	1.5	40
96	Molecular design of electron transport with orbital rule: toward conductance-decay free molecular junctions. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 32099-32110.	1.3	40
97	Computational Exploration of the Mechanism of the Hydrogenation Step of the Anthraquinone Process for Hydrogen Peroxide Production. <i>Journal of Physical Chemistry C</i> , 2015, 119, 8748-8754.	1.5	40
98	Orbital Control of Single-Molecule Conductance Perturbed by π -Accepting Anchor Groups: Cyanide and Isocyanide. <i>Journal of Physical Chemistry C</i> , 2012, 116, 20607-20616.	1.5	39
99	Selective carbon dioxide adsorption of μ -Keggin-type zirconomolybdate-based purely inorganic 3D frameworks. <i>Journal of Materials Chemistry A</i> , 2015, 3, 746-755.	5.2	39
100	A New Family of Anionic Fe ^{III} Spin Crossover Complexes Featuring a Weak π -Field N ₂ O ₄ Coordination Octahedron. <i>Chemistry - A European Journal</i> , 2016, 22, 1253-1257.	1.7	39
101	Azaferrocene-Based PNP-Type Pincer Ligand: Synthesis of Molybdenum, Chromium, and Iron Complexes and Reactivity toward Nitrogen Fixation. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 4856-4861.	1.0	39
102	Giant anisotropic thermal expansion actuated by thermodynamically assisted reorientation of imidazoliums in a single crystal. <i>Nature Communications</i> , 2019, 10, 4805.	5.8	39
103	Molecular Rectifier Based on π - π Stacked Charge Transfer Complex. <i>Journal of Physical Chemistry C</i> , 2012, 116, 2575-2580.	1.5	38
104	Disilaruthena- and Ferracyclic Complexes Containing Isocyanide Ligands as Effective Catalysts for Hydrogenation of Unfunctionalized Sterically Hindered Alkenes. <i>Journal of the American Chemical Society</i> , 2018, 140, 4119-4134.	6.6	38
105	Mechanistic Proposals for Direct Benzene Hydroxylation over Fe \rightarrow ZSM-5 Zeolite. <i>Journal of Physical Chemistry B</i> , 2003, 107, 11404-11410.	1.2	37
106	Formation and characterization of a reactive chromium(ν) \rightarrow oxo complex: mechanistic insight into hydrogen-atom transfer reactions. <i>Chemical Science</i> , 2015, 6, 945-955.	3.7	37
107	Dioxygen Activation on Cu-MOR Zeolite: Theoretical Insights into the Formation of Cu ₂ O and Cu ₃ O ₃ Active Species. <i>Inorganic Chemistry</i> , 2018, 57, 10146-10152.	1.9	37
108	Role of Hydrogen-Bonding and OH \rightarrow π Interactions in the Adhesion of Epoxy Resin on Hydrophilic Surfaces. <i>ACS Omega</i> , 2020, 5, 26211-26219.	1.6	36

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109	Quantum Transport Effects in Nanosized Graphite Sheets. II. Enhanced Transport Effects by Heteroatoms. <i>Journal of Physical Chemistry B</i> , 2003, 107, 8789-8793.	1.2	35
110	Mechanistic aspects in the direct synthesis of hydrogen peroxide on PdAu catalyst from first principles. <i>Catalysis Today</i> , 2015, 248, 142-148.	2.2	35
111	Molecular Orbital Interactions in the Nanostar Dendrimer. <i>Journal of Physical Chemistry B</i> , 2003, 107, 14204-14210.	1.2	34
112	QM/MM Study on the Catalytic Mechanism of Benzene Hydroxylation over Fe ²⁺ /ZSM-5. <i>Organometallics</i> , 2006, 25, 3118-3123.	1.1	34
113	Theoretical Study of Thermal Spin Transition between the Singlet State and the Quintet State in the [Fe(2-picolyamine) ₃] ²⁺ Spin Crossover System. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5862-5869.	1.1	34
114	A Ruthenium(III) π -Oxyl Complex Bearing Strong Radical Character. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 14041-14045.	7.2	34
115	Heterometallic Fe ^{III} /K Coordination Polymer with a Wide Thermal Hysteretic Spin Transition at Room Temperature. <i>Chemistry - A European Journal</i> , 2016, 22, 532-538.	1.7	34
116	Mechanism for the Direct Oxidation of Benzene to Phenol by FeO ⁺ . <i>Organometallics</i> , 2005, 24, 3532-3538.	1.1	33
117	Role of Acidic Proton in the Decomposition of NO over Dimeric Cu(I) Active Sites in Cu-ZSM-5 Catalyst: A QM/MM Study. <i>ACS Catalysis</i> , 2014, 4, 2075-2085.	5.5	33
118	Hydrogen atom abstraction reactions independent of C-H bond dissociation energies of organic substrates in water: significance of oxidant-substrate adduct formation. <i>Chemical Science</i> , 2014, 5, 1429-1436.	3.7	33
119	Visible light-driven cross-coupling reactions of alkyl halides with phenylacetylene derivatives for C(sp ³)-C(sp) bond formation catalyzed by a B ₁₂ complex. <i>Chemical Communications</i> , 2019, 55, 13070-13073.	2.2	33
120	Catalytic C-H amination driven by intramolecular ligand-to-nitrene one-electron transfer through a rhodium(III) centre. <i>Chemical Communications</i> , 2017, 53, 4849-4852.	2.2	32
121	Theoretical Investigation of Methane Hydroxylation over Isoelectronic [FeO] ²⁺ and [MnO] ⁺ -Exchanged Zeolites Activated by N ₂ O. <i>Inorganic Chemistry</i> , 2017, 56, 10370-10380.	1.9	32
122	The Role of Orbital Interactions in Determining the Interlayer Spacing in Graphite Slabs. <i>Journal of the American Chemical Society</i> , 2000, 122, 11871-11875.	6.6	31
123	Mechanism for the Formaldehyde to Formic Acid and the Formic Acid to Carbon Dioxide Conversions Mediated by an Iron-Oxo Species. <i>Journal of Physical Chemistry A</i> , 2002, 106, 621-630.	1.1	31
124	Reverse Exponential Decay of Electrical Transmission in Nanosized Graphite Sheets. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7565-7572.	1.2	31
125	Intraprotein transmethylation via a CH ₃ -Co(III) species in myoglobin reconstituted with a cobalt corrinoid complex. <i>Dalton Transactions</i> , 2016, 45, 3277-3284.	1.6	31
126	Theoretical Measurements of Conductance in an (AT) ₁₂ DNA Molecule. <i>ChemPhysChem</i> , 2003, 4, 1256-1260.	1.0	30

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127	Anisotropic Change in the Magnetic Susceptibility of a Dynamic Single Crystal of a Cobalt(II) Complex. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 717-721.	7.2	30
128	DFT exploration of active site motifs in methane hydroxylation by Ni-ZSM-5 zeolite. <i>Catalysis Science and Technology</i> , 2018, 8, 5875-5885.	2.1	30
129	Mechanistic Insight into Concerted Proton-Electron Transfer of a Ru(IV)-Oxo Complex: A Possible Oxidative Asynchronicity. <i>Journal of the American Chemical Society</i> , 2020, 142, 16982-16989.	6.6	30
130	DFT Study on N ₂ Activation by a Hydride-Bridged Diniobium Complex. N≡N Bond Cleavage Accompanied by H ₂ Evolution. <i>Inorganic Chemistry</i> , 2009, 48, 3875-3881.	1.9	29
131	Current Rectification through π - π Stacking in Multilayered Donor-Acceptor Cyclophanes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 26625-26635.	1.5	28
132	Possible Peroxo State of the Dicopper Site of Particulate Methane Monooxygenase from Combined Quantum Mechanics and Molecular Mechanics Calculations. <i>Inorganic Chemistry</i> , 2016, 55, 2771-2775.	1.9	28
133	Frontier Orbital Perspective for Quantum Interference in Alternant and Nonalternant Hydrocarbons. <i>Journal of Physical Chemistry C</i> , 2017, 121, 9621-9626.	1.5	28
134	Synthesis and reactivity of titanium- and zirconium-dinitrogen complexes bearing anionic pyrrole-based PNP-type pincer ligands. <i>Dalton Transactions</i> , 2018, 47, 11322-11326.	1.6	28
135	Quenching and Restoration of Orbital Angular Momentum through a Dynamic Bond in a Cobalt(II) Complex. <i>Journal of the American Chemical Society</i> , 2020, 142, 11434-11441.	6.6	28
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