Kazunari Yoshizawa

List of Publications by Year in descending order

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331 papers

13,148 citations

63 h-index 97 g-index

342 all docs 342 docs citations

times ranked

342

10229 citing authors

#	Article	IF	CITATIONS
1	Exploring Metal Cluster Catalysts Using Swarm Intelligence: Start with Hydrogen Adsorption. Topics in Catalysis, 2022, 65, 215-227.	1.3	2
2	Cubically cage-shaped mesoporous ordered silica for simultaneous visual detection and removal of uranium ions from contaminated seawater. Mikrochimica Acta, 2022, 189, 3.	2.5	7
3	Halide-Adducts of OsO4. Structure and Reactivity in Alcohol-Oxidation. Bulletin of the Chemical Society of Japan, 2022, 95, 64-72.	2.0	5
4	Topology Dictates Magnetic and Conductive Properties of a π-Stacked System: Insight into Possible Coexistence of Magnetic and Conductive Systems. Journal of Physical Chemistry C, 2022, 126, 3244-3256.	1.5	3
5	C(sp ³)–H bond activation by the carboxylate-adduct of osmium tetroxide (OsO ₄). Dalton Transactions, 2022, 51, 1123-1130.	1.6	4
6	Augmented Selfâ€Association by Electrostatic Forces in Thienopyrroleâ€Fused Thiadiazoles that Contain an Ester instead of an Ether Linker. Chemistry - an Asian Journal, 2022, 17, .	1.7	0
7	Graph-theoretical exploration of the relation between conductivity and connectivity in heteroatom-containing single-molecule junctions. Journal of Chemical Physics, 2022, 156, 091102.	1.2	2
8	Mechanistic study on reduction of nitric oxide to nitrous oxide using a dicopper complex. Dalton Transactions, 2022, 51, 5399-5403.	1.6	1
9	Synthesis, redox properties, and catalytic hydrogen gas generation of porphycene cobalt complexes. Journal of Porphyrins and Phthalocyanines, 2022, 26, 263-272.	0.4	1
10	Catalytic Reduction of Dinitrogen into Ammonia and Hydrazine by Using Chromium Complexes Bearing PCPâ€Type Pincer Ligands**. Chemistry - A European Journal, 2022, 28, .	1.7	13
11	Catalytic Reduction of Dinitrogen to Ammonia and Hydrazine Using Iron–Dinitrogen Complexes Bearing Anionic Benzene-Based PCP-Type Pincer Ligands. Bulletin of the Chemical Society of Japan, 2022, 95, 683-692.	2.0	11
12	Synthesis and Reactivity of Cobalt–Dinitrogen Complexes Bearing Anionic PCP-Type Pincer Ligands toward Catalytic Silylamine Formation from Dinitrogen. Inorganic Chemistry, 2022, 61, 5190-5195.	1.9	8
13	Hydroboration and Hydrosilylation of a Molybdenum–Nitride Complex Bearing a PNP-Type Pincer Ligand. Organometallics, 2022, 41, 366-373.	1.1	5
14	Theoretical Investigation into Selective Benzene Hydroxylation by Ruthenium-Substituted Keggin-Type Polyoxometalates. Inorganic Chemistry, 2022, 61, 10-14.	1.9	2
15	Heterointerface Created on Auâ€Clusterâ€Loaded Unilamellar Hydroxide Electrocatalysts as a Highly Active Site for the Oxygen Evolution Reaction (Adv. Mater. 16/2022). Advanced Materials, 2022, 34, .	11.1	1
16	Light-driven oxidation of CH ₄ to C ₁ chemicals catalysed by an organometallic Ru complex with O ₂ . RSC Advances, 2022, 12, 12253-12257.	1.7	3
17	Peel Adhesion Strength between Epoxy Resin and Hydrated Silica Surfaces: A Density Functional Theory Study. ACS Omega, 2022, 7, 17393-17400.	1.6	8
18	Theoretical Study on the Contribution of Interfacial Functional Groups to the Adhesive Interaction between Epoxy Resins and Aluminum Surfaces. Langmuir, 2022, 38, 6653-6664.	1.6	19

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19	Mechanistic Study for the Reaction of B ₁₂ Complexes with <i>m</i> Acid in Catalytic Alkane Oxidations. Inorganic Chemistry, 2022, 61, 9710-9724.	1.9	11
20	Attenuation of Redox Switching and Rectification in Azulenequinones/Hydroquinones after B and N Doping: A Firstâ€Principles Investigation. Advanced Theory and Simulations, 2021, 4, 2000203.	1.3	2
21	Arylene–hexaynylene and –octaynylene macrocycles: extending the polyyne chains drives self-association by enhanced dispersion force. Chemical Communications, 2021, 57, 576-579.	2.2	3
22	Oxygen Atom Insertion into the Osmium–Carbon Bond via an Organometallic Oxido–Osmium(V) Intermediate. Organometallics, 2021, 40, 102-106.	1.1	7
23	Bonding of C ₁ fragments on metal nanoclusters: a search for methane conversion catalysts with swarm intelligence. Physical Chemistry Chemical Physics, 2021, 23, 14004-14015.	1.3	12
24	From Infection Clusters to Metal Clusters: Significance of the Lowest Occupied Molecular Orbital (LOMO). ACS Omega, 2021, 6, 1339-1351.	1.6	6
25	Electronic Origin of Catalytic Activity of TiH ₂ for Ammonia Synthesis. Journal of Physical Chemistry C, 2021, 125, 3948-3960.	1.5	13
26	Theoretical Study on the Adhesion Interaction between Epoxy Resin Including Curing Agent and Plated Gold Surface. Langmuir, 2021, 37, 3982-3995.	1.6	18
27	Mechanistic Insights into the Dicopper-Complex-Catalyzed Hydroxylation of Methane and Benzene Using Nitric Oxide: A DFT Study. Inorganic Chemistry, 2021, 60, 4599-4609.	1.9	4
28	Synthesis, spectral characterization, density functional theory studies, and biological screening of some transition metal complexes of a novel hydrazide–hydrazone ligand of isonicotinic acid. Applied Organometallic Chemistry, 2021, 35, e6205.	1.7	20
29	One-Pot Synthesis of Tertiary Amides from Organic Trichlorides through Oxygen Atom Incorporation from Air by Convergent Paired Electrolysis. Journal of Organic Chemistry, 2021, 86, 5983-5990.	1.7	20
30	Mixed Anion Control of the Partial Oxidation of Methane to Methanol on the β-PtO ₂ Surface. ACS Omega, 2021, 6, 13858-13869.	1.6	9
31	Ammonia Formation Catalyzed by a Dinitrogenâ€Bridged Dirhenium Complex Bearing PNPâ€Pincer Ligands under Mild Reaction Conditions**. Angewandte Chemie - International Edition, 2021, 60, 13906-13912.	7.2	21
32	Ammonia Formation Catalyzed by a Dinitrogenâ€Bridged Dirhenium Complex Bearing PNPâ€Pincer Ligands under Mild Reaction Conditions**. Angewandte Chemie, 2021, 133, 14025-14031.	1.6	2
33	Effect of chemically induced permittivity changes on the plasmonic properties of metal nanoparticles. Communications Materials, 2021, 2, .	2.9	5
34	Electrochemical Synthesis of Cyanoformamides from Trichloroacetonitrile and Secondary Amines Mediated by the B12 Derivative. Journal of Organic Chemistry, 2021, 86, 16134-16143.	1.7	8
35	Quadruple Role of Pd Catalyst in Domino Reaction Involving Aryl to Alkyl 1,5â€Pd Migration to Access 1,9â€Bridged Triptycenes. Chemistry - A European Journal, 2021, 27, 11548-11553.	1.7	7
36	Energy Decomposition Analysis of the Adhesive Interaction between an Epoxy Resin Layer and a Silica Surface. Langmuir, 2021, 37, 8417-8425.	1.6	15

3

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37	Distinct Behaviors of Cu- and Ni-ZSM-5 Zeolites toward the Post-activation Reactions of Methane. Journal of Physical Chemistry C, 2021, 125, 19333-19344.	1.5	6
38	Manipulating electron redistribution to achieve electronic pyroelectricity in molecular [FeCo] crystals. Nature Communications, 2021, 12, 4836.	5.8	21
39	S,C,C- and O,C,C-Bridged Triarylamines and Their Persistent Radical Cations. Journal of Organic Chemistry, 2021, 86, 12559-12568.	1.7	8
40	Competition between Hydrogen Bonding and Dispersion Force in Water Adsorption and Epoxy Adhesion to Boron Nitride: From the Flat to the Curved. Langmuir, 2021, 37, 11351-11364.	1.6	17
41	Theoretical Views on Catalytic Reaction Pathways for Nitrogen Fixation by Dinitrogen-Bridging Dimolybdenum Complexes. Yuki Gosei Kagaku Kyokaishi/Journal of Synthetic Organic Chemistry, 2021, 79, 1041-1049.	0.0	1
42	Tin(II)â€"Nitrene Radical Complexes Formed by Electron Transfer from Redox-Active Ligand to Organic Azides and Their Reactivity in C(sp ³)â€"H Activation. Inorganic Chemistry, 2021, 60, 18603-18607.	1.9	6
43	Elucidation of Adhesive Interaction between the Epoxy Molding Compound and Cu Lead Frames. ACS Omega, 2021, 6, 34173-34184.	1.6	13
44	Molecular Dynamics Study on the Thermal Aspects of the Effect of Water Molecules at the Adhesive Interface on an Adhesive Structure. Langmuir, 2021, 37, 14724-14732.	1.6	7
45	Mechanistic Study on Catalytic Disproportionation of Hydrazine by a Protic Pincerâ€Type Iron Complex through Protonâ€Coupled Electron Transfer. European Journal of Inorganic Chemistry, 2020, 2020, 1472-1482.	1.0	8
46	Nitrogen Fixation Catalyzed by Dinitrogenâ€Bridged Dimolybdenum Complexes Bearing PCP―and PNPâ€Type Pincer Ligands: A Shortcut Pathway Deduced from Free Energy Profiles. European Journal of Inorganic Chemistry, 2020, 2020, 1490-1498.	1.0	17
47	Computational Study on the Light-Induced Oxidation of Iridium–Aqua Complex to Iridium–Oxo Complex over WO ₃ (001) Surface. Inorganic Chemistry, 2020, 59, 415-422.	1.9	4
48	Mechanistic Study on Ring ontracting Skeletal Rearrangement from Porphycene to Isocorrole by Experimental and Theoretical Methods. European Journal of Organic Chemistry, 2020, 2020, 1811-1816.	1.2	2
49	Theoretical Study on the Electronic Structure of Heavy Alkali-Metal Suboxides. Inorganic Chemistry, 2020, 59, 1340-1354.	1.9	10
50	Cycling between Molybdenumâ€Dinitrogen and â€Nitride Complexes to Support the Reaction Pathway for Catalytic Formation of Ammonia from Dinitrogen. Chemistry - A European Journal, 2020, 26, 13321-13321.	1.7	4
51	Role of Hydrogen-Bonding and OHâ^'Ï€ Interactions in the Adhesion of Epoxy Resin on Hydrophilic Surfaces. ACS Omega, 2020, 5, 26211-26219.	1.6	36
52	Mixed-Anion Control of C–H Bond Activation of Methane on the IrO2 Surface. Journal of Physical Chemistry C, 2020, 124, 17058-17072.	1.5	13
53	Photocatalytic hydrogen evolution using a Ru(ii)-bound heteroaromatic ligand as a reactive site. Dalton Transactions, 2020, 49, 17230-17242.	1.6	11
54	Selective catalytic 2e ^{â^'} -oxidation of organic substrates by an Fe ^{II} complex having an N-heterocyclic carbene ligand in water. Chemical Communications, 2020, 56, 9783-9786.	2.2	8

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55	Redox properties of a bipyrimidine-bridged dinuclear ruthenium(II) complex. Inorganic Chemistry Communication, 2020, 120, 108150.	1.8	1
56	Molecular functionalization of all-inorganic perovskite CsPbBr ₃ thin films. Journal of Materials Chemistry C, 2020, 8, 12587-12598.	2.7	3
57	Novel Mechanistic Insights into Methane Activation over Fe and Cu Active Sites in Zeolites: A Comparative DFT Study Using Meta-GGA Functionals. Journal of Physical Chemistry C, 2020, 124, 1812-18125.	1.5	24
58	Electronic and Optical Modulation of Metal-Doped Hybrid Organic–Inorganic Perovskites Crystals by Post-Treatment Control. ACS Applied Energy Materials, 2020, 3, 7500-7511.	2.5	10
59	Mechanical Control of Molecular Conductance and Diradical Character in Bond Stretching and π-Stack Compression. Journal of Physical Chemistry C, 2020, 124, 22941-22958.	1.5	9
60	Comparative study of the ideal and actual adhesion interfaces of the die bonding structure using conductive adhesives. Journal of Adhesion, 2020, , 1-25.	1.8	10
61	Mechanistic Insight into Concerted Proton–Electron Transfer of a Ru(IV)-Oxo Complex: A Possible Oxidative Asynchronicity. Journal of the American Chemical Society, 2020, 142, 16982-16989.	6.6	30
62	Macroscopic Polarization Change via Electron Transfer in a Valence Tautomeric Cobalt Complex. Nature Communications, 2020, 11, 1992.	5.8	41
63	Threeâ€Step Spin State Transition and Hysteretic Proton Transfer in the Crystal of an Iron(II) Hydrazone Complex. Angewandte Chemie, 2020, 132, 14891-14897.	1.6	4
64	Threeâ€Step Spin State Transition and Hysteretic Proton Transfer in the Crystal of an Iron(II) Hydrazone Complex. Angewandte Chemie - International Edition, 2020, 59, 14781-14787.	7.2	15
65	Iridium-catalyzed Formation of Silylamine from Dinitrogen under Ambient Reaction Conditions. Chemistry Letters, 2020, 49, 794-797.	0.7	9
66	Theoretical Study of the Direct Conversion of Methane to Methanol Using H ₂ O ₂ as an Oxidant on Pd and Au/Pd Surfaces. Journal of Physical Chemistry C, 2020, 124, 13231-13239.	1.5	17
67	Cycling between Molybdenumâ€Dinitrogen and â€Nitride Complexes to Support the Reaction Pathway for Catalytic Formation of Ammonia from Dinitrogen. Chemistry - A European Journal, 2020, 26, 13383-13389.	1.7	25
68	Quenching and Restoration of Orbital Angular Momentum through a Dynamic Bond in a Cobalt(II) Complex. Journal of the American Chemical Society, 2020, 142, 11434-11441.	6.6	28
69	Chemical transformations of push–pull fluorenones: push–pull dibenzodicyanofulvenes as well as fluorenone– and dibenzodicyanofulvene–tetracyanobutadiene conjugates. Organic and Biomolecular Chemistry, 2020, 18, 4198-4209.	1.5	4
70	Active Catalyst for Methane Hydroxylation by an Iridium–Oxo Complex. ACS Catalysis, 2020, 10, 8254-8262.	5.5	4
71	Local Structures and Dynamics of Imidazole Molecules in Poly(vinylphosphonic acid)–Imidazole Composite Investigated by Molecular Dynamics. ACS Applied Polymer Materials, 2020, 2, 1561-1568.	2.0	11
72	Room-Temperature Activation of Methane and Direct Formations of Acetic Acid and Methanol on Zn-ZSM-5 Zeolite: A Mechanistic DFT Study. Bulletin of the Chemical Society of Japan, 2020, 93, 345-354.	2.0	21

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73	Understanding Single-Molecule Parallel Circuits on the Basis of Frontier Orbital Theory. Journal of Physical Chemistry C, 2020, 124, 3322-3331.	1.5	11
74	Structural characterization of molybdenum–dinitrogen complex as key species toward ammonia formation by dispersive XAFS spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 12368-12372.	1.3	9
75	Theoretical rationalization for the equilibrium between (μâ€'η ² :η ² -peroxido)Cu ^{II} Cu ^{II} and bis(μ-oxido)Cu ^{III} Cu ^{III} complexes: perturbational effects from ligand frameworks. Dalton Transactions. 2020. 49. 6710-6717.	1.6	3
76	Optimization of Work Function via Bayesian Machine Learning Combined with First-Principles Calculation. Journal of Physical Chemistry C, 2020, 124, 9958-9970.	1.5	27
77	Anthranoxides as Highly Reactive Arynophiles for the Synthesis of Triptycenes. Chemistry - A European Journal, 2020, 26, 8506-8510.	1.7	10
78	Mechanistic Understanding of Methane Hydroxylation by Cu-Exchanged Zeolites., 2020,, 75-86.		1
79	Dynamics and Energetics of Methane on the Surfaces of Transition Metal Oxides. , 2020, , 101-133.		2
80	Preparation and reactivity of molybdenum complexes bearing pyrrole-based PNP-type pincer ligand. Chemical Communications, 2020, 56, 6933-6936.	2.2	17
81	Osmotic pressure effects identify dehydration upon cytochrome c–cytochrome c oxidase complex formation contributing to a specific electron pathway formation. Biochemical Journal, 2020, 477, 1565-1578.	1.7	3
82	Theoretical Study of Methanol Oxidation by Ni-ZSM-5. Journal of Computer Chemistry Japan, 2020, 19, 151-153.	0.0	0
83	Theoretical Suggestion of a Methane Hydroxylation Catalyst. Journal of Computer Chemistry Japan, 2020, 19, 133-135.	0.0	0
84	Orbital Concept for Methane Activation. , 2020, , 1-22.		0
85	Esterification of Tertiary Amides by Alcohols Through Câ^'N Bond Cleavage over CeO ₂ . ChemCatChem, 2019, 11, 449-456.	1.8	21
86	Observation of Proton Transfer Coupled Spin Transition and Trapping of Photoinduced Metastable Proton Transfer State in an Fe(II) Complex. Journal of the American Chemical Society, 2019, 141, 14384-14393.	6.6	23
87	Fundamental electron-transfer and proton-coupled electron-transfer properties of Ru(iv)-oxo complexes. Dalton Transactions, 2019, 48, 13154-13161.	1.6	12
88	Electronic transport investigation of redox-switching of azulenequinones/hydroquinones <i>via</i> first-principles studies. Physical Chemistry Chemical Physics, 2019, 21, 17859-17867.	1.3	2
89	Giant anisotropic thermal expansion actuated by thermodynamically assisted reorientation of imidazoliums in a single crystal. Nature Communications, 2019, 10, 4805.	5.8	39
90	Computational Studies on the Thermodynamic and Kinetic Parameters of Oxidation of 2-Methoxyethanol Biofuel via H-Atom Abstraction by Methyl Radical. Scientific Reports, 2019, 9, 15361.	1.6	17

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91	Role of Amino Acid Residues for Dioxygen Activation in the Second Coordination Sphere of the Dicopper Site of pMMO. Inorganic Chemistry, 2019, 58, 12280-12288.	1.9	8
92	Mechanistic Insights into Methane Oxidation by Molecular Oxygen under Photoirradiation: Controlled Radical Chain Reactions. Bulletin of the Chemical Society of Japan, 2019, 92, 1840-1846.	2.0	1
93	An Azulene-Based Chiral Helicene and Its Air-Stable Cation Radical. Bulletin of the Chemical Society of Japan, 2019, 92, 1867-1873.	2.0	21
94	Formation of a Ruthenium(V)â€"Imido Complex and the Reactivity in Substrate Oxidation in Water through the Nitrogen Non-Rebound Mechanism. Inorganic Chemistry, 2019, 58, 12815-12824.	1.9	8
95	Cupric-superoxide complex that induces a catalytic aldol reaction-type C–C bond formation. Communications Chemistry, 2019, 2, .	2.0	19
96	Synthesis and Catalytic Reactivity of Bis(molybdenum-trihalide) Complexes Bridged by Ferrocene Skeleton toward Catalytic Nitrogen Fixation. Organometallics, 2019, 38, 2863-2872.	1.1	13
97	Molybdenum-Catalyzed Ammonia Formation Using Simple Monodentate and Bidentate Phosphines as Auxiliary Ligands. Inorganic Chemistry, 2019, 58, 8927-8932.	1.9	48
98	Lithium-Richest Phase of Lithium Tetrelides Li17Tt4 (Tt = Si, Ge, Sn, and Pb) as an Electride. Bulletin of the Chemical Society of Japan, 2019, 92, 1154-1169.	2.0	16
99	Dual Catalytic Cycle of H2 and H2O Oxidations by a Half-Sandwich Iridium Complex: A Theoretical Study. Inorganic Chemistry, 2019, 58, 7274-7284.	1.9	4
100	Prediction of the Glass-Transition Temperatures of Linear Homo/Heteropolymers and Cross-Linked Epoxy Resins. ACS Applied Polymer Materials, 2019, 1, 1430-1442.	2.0	25
101	Methane selective oxidation to methanol by metal-exchanged zeolites: a review of active sites and their reactivity. Catalysis Science and Technology, 2019, 9, 1744-1768.	2.1	148
102	Thermochemistry and Kinetics of the Thermal Degradation of 2-Methoxyethanol as Possible Biofuel Additives. Scientific Reports, 2019, 9, 4535.	1.6	20
103	Adhesion of Epoxy Resin with Hexagonal Boron Nitride and Graphite. ACS Omega, 2019, 4, 4491-4504.	1.6	43
104	Methane Activation at the Metal–Support Interface of Ni ₄ –CeO ₂ (111) Catalyst: A Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 9788-9798.	1.5	48
105	Catalytic Reactivity of Molybdenum–Trihalide Complexes Bearing PCPâ€Type Pincer Ligands. Chemistry - an Asian Journal, 2019, 14, 2091-2096.	1.7	24
106	High-Temperature Cooperative Spin Crossover Transitions and Single-Crystal Reflection Spectra of [FellI(qsal)2](CH3OSO3) and Related Compounds. Crystals, 2019, 9, 81.	1.0	11
107	Catalytic reduction of dinitrogen to tris(trimethylsilyl)amine using rhodium complexes with a pyrrole-based PNP-type pincer ligand. Chemical Communications, 2019, 55, 14886-14889.	2.2	26
108	Real-space observation of far- and near-field-induced photolysis of molecular oxygen on an Ag(110) surface by visible light. Journal of Chemical Physics, 2019, 151, 144705.	1.2	14

7

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109	Temperature dependence of spherical electron transfer in a nanosized [Fe14] complex. Nature Communications, 2019, 10, 5510.	5.8	12
110	Visible light-driven cross-coupling reactions of alkyl halides with phenylacetylene derivatives for C(sp ³)â€"C(sp) bond formation catalyzed by a B ₁₂ complex. Chemical Communications, 2019, 55, 13070-13073.	2.2	33
111	Esterification of Tertiary Amides by Alcohols Through Câ^'N Bond Cleavage over CeO 2. ChemCatChem, 2019, 11, 15-15.	1.8	0
112	Molecular understanding of the adhesive interactions between silica surface and epoxy resin: Effects of interfacial water. Journal of Computational Chemistry, 2019, 40, 164-171.	1.5	45
113	Redox behaviour of the \hat{l}^2 -dihydroporphycene cobalt complex: study on the effect of hydrogenation of the ligand. Dalton Transactions, 2019, 48, 872-881.	1.6	4
114	Theoretical Study on the Relation between the Frontier Orbital and the Conductance in Aromatic Single-Molecular Parallel Circuits. Journal of Computer Chemistry Japan, 2019, 18, 227-229.	0.0	0
115	Disilaruthena- and Ferracyclic Complexes Containing Isocyanide Ligands as Effective Catalysts for Hydrogenation of Unfunctionalized Sterically Hindered Alkenes. Journal of the American Chemical Society, 2018, 140, 4119-4134.	6.6	38
116	Catalytic Reduction of Molecular Dinitrogen to Ammonia and Hydrazine Using Vanadium Complexes. Angewandte Chemie, 2018, 130, 9202-9206.	1.6	20
117	Trithiazolyl-1,3,5-triazines bearing decyloxybenzene moieties: synthesis, photophysical and electrochemical properties, and self-assembly behavior. Organic and Biomolecular Chemistry, 2018, 16, 3584-3595.	1.5	8
118	Catalytic Reduction of Molecular Dinitrogen to Ammonia and Hydrazine Using Vanadium Complexes. Angewandte Chemie - International Edition, 2018, 57, 9064-9068.	7.2	109
119	Cobalt–Carbon Bond Formation Reaction via Ligand Reduction of Porphycene–Cobalt(II) Complex and Its Noninnocent Reactivity. ACS Omega, 2018, 3, 4027-4034.	1.6	17
120	Methane Partial Oxidation over [Cu ₂ (î½-O)] ²⁺ and [Cu ₃ (î½-O) ₃] ²⁺ Active Species in Large-Pore Zeolites. ACS Catalysis, 2018, 8, 1500-1509.	5. 5	104
121	Contribution of Coulomb Interactions to a Two-Step Crystal Structure Phase Transformation Coupled with a Significant Change in Spin Crossover Behavior for a Series of Charged Fe ^{II} Complexes from 2,6-Bis(2-methylthiazol-4-yl)pyridine. Inorganic Chemistry, 2018, 57, 1277-1287.	1.9	17
122	Two Discrete RuCp* (Cp*=Pentamethylcyclopentadienyl) Binding Modes of Nâ€Confused Porphyrins: Peripheral π Complex and Sitting Atop Ruthenocenophane Complex by Skeletal Transformation. Chemistry - A European Journal, 2018, 24, 6742-6746.	1.7	5
123	Intermediate-Spin Iron(III) Complexes Having a Redox-Noninnocent Macrocyclic Tetraamido Ligand. Inorganic Chemistry, 2018, 57, 9683-9695.	1.9	13
124	Combined theoretical and experimental study on alcoholysis of amides on CeO2 surface: A catalytic interplay between Lewis acid and base sites. Catalysis Today, 2018, 303, 256-262.	2.2	13
125	NH Tautomerism of a Quadruply Fused Porphyrin: Rigid Fused Structure Delays the Proton Transfer. Journal of Physical Chemistry B, 2018, 122, 316-327.	1.2	2
126	Catalytic Performance of a Dicopper–Oxo Complex for Methane Hydroxylation. Inorganic Chemistry, 2018, 57, 8-11.	1.9	20

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127	Formation and Isolation of a Fourâ€Electronâ€Reduced Porphyrin Derivative by Reduction of a Stable 20Ï€ Isophlorin. Angewandte Chemie - International Edition, 2018, 57, 1973-1977.	7.2	10
128	DFT exploration of active site motifs in methane hydroxylation by Ni-ZSM-5 zeolite. Catalysis Science and Technology, 2018, 8, 5875-5885.	2.1	30
129	Interaction of SrO-terminated SrTiO ₃ surface with oxygen, carbon dioxide, and water. Journal of Materials Chemistry A, 2018, 6, 22662-22672.	5.2	24
130	A Study of Adhesion Interface about Die Bonding Structure with Conductive Silver Paste., 2018,,.		4
131	Density-Functional Tight-Binding Study on the Effects of Interfacial Water in the Adhesion Force between Epoxy Resin and Alumina Surface. Langmuir, 2018, 34, 14428-14438.	1.6	27
132	Effects of electron-phonon coupling on quantum interference in polyenes. Journal of Chemical Physics, 2018, 149, 134115.	1.2	6
133	Importance of the Reactant-State Potentials of Chromium(V)–Oxo Complexes to Determine the Reactivity in Hydrogen-Atom Transfer Reactions. Inorganic Chemistry, 2018, 57, 13929-13936.	1.9	8
134	Theoretical Overview of Methane Hydroxylation by Copper–Oxygen Species in Enzymatic and Zeolitic Catalysts. Accounts of Chemical Research, 2018, 51, 2382-2390.	7.6	85
135	Mechanistic Insights into Homogeneous Electrocatalytic and Photocatalytic Hydrogen Evolution Catalyzed by High-Spin Ni(II) Complexes with S ₂ N ₂ -Type Tetradentate Ligands. Inorganic Chemistry, 2018, 57, 7180-7190.	1.9	47
136	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
137	Synthesis and reactivity of titanium- and zirconium-dinitrogen complexes bearing anionic pyrrole-based PNP-type pincer ligands. Dalton Transactions, 2018, 47, 11322-11326.	1.6	28
138	Ground-State Copper(III) Stabilized by N-Confused/N-Linked Corroles: Synthesis, Characterization, and Redox Reactivity. Journal of the American Chemical Society, 2018, 140, 6883-6892.	6.6	45
139	Dioxygen Activation on Cu-MOR Zeolite: Theoretical Insights into the Formation of Cu ₂ O and Cu ₃ O ₃ Active Species. Inorganic Chemistry, 2018, 57, 10146-10152.	1.9	37
140	Aerobic oxidation of alkanes on icosahedron gold nanoparticle Au55. Journal of Catalysis, 2018, 364, 141-153.	3.1	9
141	Electrical Conductance and Diode-Like Behavior of Substituted Azulene. Journal of Physical Chemistry C, 2017, 121, 2504-2511.	1.5	13
142	<i>i) $f < i\rangle$-CAM Mechanisms for the Hydrogenation of Alkenes by <i>cis</i>- and <i>trans</i>- Disilametallacyclic Carbonyl Complexes (M = Fe, Ru, Os): Experimental and Theoretical Studies. Bulletin of the Chemical Society of Japan, 2017, 90, 613-626.</i>	2.0	9
143	Redox Potentials of Cobalt Corrinoids with Axial Ligands Correlate with Heterolytic Co–C Bond Dissociation Energies. Inorganic Chemistry, 2017, 56, 1950-1955.	1.9	22
144	Thermodynamics and Photodynamics of a Monoprotonated Porphyrin Directly Stabilized by Hydrogen Bonding with Polar Protic Solvents. Chemistry - A European Journal, 2017, 23, 4669-4679.	1.7	13

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