Shigeyoshi Sakaki

List of Publications by Year
in descending order

188	7,109	57758 44	71685 76
papers	citations	h-index	g-index

193	193	193	6591
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Rh Complex with Unique Rhâ€“Al Direct Bond: Theoretical Insight into its Characteristic Features and Application to Catalytic Reaction via Ïƒ-Bond Activation. Topics in Catalysis, 2022, 65, 392-417.	2.8	7
2	Molecule in soft-crystal at ground and excited states: Theoretical approach. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2022, 51, 100482.	11.6	5
3	Theoretical Study on Siâ^'Cl Bond Activation in Pdâ€Catalyzed Crossâ€Coupling of Chlorosilanes with Organoaluminum. European Journal of Organic Chemistry, 2022, 2022, .	2.4	7
4	Single atom alloys vs. phase separated alloys in Cu, Ag, and Au atoms with Ni(111) and Ni, Pd, and Pt atoms with Cu(111): a theoretical exploration. Physical Chemistry Chemical Physics, 2022, 24, 10420-10438.	2.8	4
5	Theoretical Insight into Catalysis of the Aluminabenzeneâ€“Iridium Complex for C(sp³)â€“H Borylation of NEt₃: How to Control Î±- and Î²-Regioselectivities?. ACS Catalysis, 2022, 12, 4880-4897.	11.2	5
6	Tunable acetylene sorption by flexible catenated metalâ€“organic frameworks. Nature Chemistry, 2022, 14, 816-822.	13.6	62
7	Theoretical Study of Nâ€“H Ïƒ-Bond Activation by Nickel(0) Complex: Reaction Mechanism, Electronic Processes, and Prediction of Better Ligand. Inorganic Chemistry, 2022, 61, 8715-8728.	4.0	2
8	Four-Electron Reduction of Dioxygen on a Metal Surface: Models of Dissociative and Associative Mechanisms in a Homogeneous System. Inorganic Chemistry, 2021, 60, 1550-1560.	4.0	1
9	Theoretical insight into oxidation catalysis of chromite spinel MCr2O4 (MÂ=ÂMg, Co, Cu, and Zn): Volcano plot for oxygen-vacancy formation and catalytic activity. Journal of Catalysis, 2021, 393, 30-41.	6.2	11
10	Deacylative Carbonâ€Carbon Bond Cleavage of Ketone Equivalents: Applications to Radical Carbonâ€Carbon Bond Formation Reactions. Chemistry - an Asian Journal, 2021, 16, 282-286.	3.3	2
11	Metal-free approach for hindered amide-bond formation with hypervalent iodine(<scp>iii</scp>) reagents: application to hindered peptide synthesis. Green Chemistry, 2021, 23, 848-855.	9.0	18
12	Theoretical Study of NO Dissociative Adsorption onto 3d Metal Particles M₅₅ (M = Fe, Co,) Tj ETQq0 0 0 rgBT /Overlock 10 ACS Omega, 2021, 6, 4888-4898.	3.5	5
13	Hostâ€“Guest Interaction Modulation in Porous Coordination Polymers for Inverse Selective CO₂/C₂H₂Separation. Angewandte Chemie, 2021, 133, 11794-11800.	2.0	18
14	Hostâ€“Guest Interaction Modulation in Porous Coordination Polymers for Inverse Selective CO₂/C₂H₂Separation. Angewandte Chemie - International Edition, 2021, 60, 11688-11694.	13.8	115
15	Catalysis of core-shell nanoparticle M@Pt (M Co and Ni) for oxygen reduction reaction and its electronic structure in comparison to Pt nanoparticle. Journal of Catalysis, 2021, 397, 13-26.	6.2	13
16	Frontispiz: Hostâ€“Guest Interaction Modulation in Porous Coordination Polymers for Inverse Selective CO₂/C₂H₂ Separation. Angewandte Chemie, 2021, 133, .	2.0	0
17	Frontispiece: Hostâ€“Guest Interaction Modulation in Porous Coordination Polymers for Inverse Selective CO₂/C₂H₂ Separation. Angewandte Chemie - International Edition, 2021, 60, .	13.8	0
18	Synthesis, Electronic Properties, and Lewis Acidity of Rhodium Complexes Bearing X-Type PBP, PAlP, and PGaP Pincer Ligands. Bulletin of the Chemical Society of Japan, 2021, 94, 1859-1868.	3.2	10

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19	C(sp³)â€“F Bond Activation and Hydrodefluorination of the CF₃ Group Catalyzed by a Nickel(II) Hydride Complex: Theoretical Insight into the Mechanism with a Spin-State Change and Two Ion-Pair Intermediates. ACS Catalysis, 2021, 11, 10681-10693.	11.2	5
20	C2-selective alkylation of pyridines by rhodiumâ€“aluminum complexes. Tetrahedron, 2021, 95, 132339.	1.9	19
21	Theoretical Study of the Propene Combustion Catalysis of Chromite Spinels: Reaction Mechanism and Relation between the Activity and Electronic Structure of Spinels. Journal of Physical Chemistry C, 2021, 125, 25983-26002.	3.1	3
22	A Dualâ€Ligand Porous Coordination Polymer Chemiresistor with Modulated Conductivity and Porosity. Angewandte Chemie - International Edition, 2020, 59, 172-176.	13.8	124
23	A Dualâ€Ligand Porous Coordination Polymer Chemiresistor with Modulated Conductivity and Porosity. Angewandte Chemie, 2020, 132, 178-182.	2.0	8
24	Aurophilicityâ€Mediated Construction of Emissive Porous Molecular Crystals as Versatile Hosts for Liquid and Solid Guests. Chemistry - A European Journal, 2020, 26, 735-744.	3.3	19
25	Coordination Flexibility of the Rh(PXP) Complex to NH₃, CO, and C₂H₄ (PXP = Diphosphine-Based Pincer Ligand; X = B, Al, and Ga): Theoretical Insight. Inorganic Chemistry, 2020, 59, 15862-15876.	4.0	9
26	O₂activation by coreâ€“shell Ru₁₃@Pt₄₂particles in comparison with Pt₅₅particles: a DFT study. RSC Advances, 2020, 10, 36090-36100.	3.6	3
27	Fluorosilane Activation by Pd/Niâ†'Siâ€“Fâ†'Lewis Acid Interaction: An Entry to Catalytic Sila-Negishi Coupling. Journal of the American Chemical Society, 2020, 142, 14039-14044.	13.7	33
28	Control of local flexibility towards p-xylene sieving in Hofmann-type porous coordination polymers. Chemical Communications, 2020, 56, 9632-9635.	4.1	14
29	Methane Borylation Catalyzed by Ru, Rh, and Ir Complexes in Comparison with Cyclohexane Borylation: Theoretical Understanding and Prediction. Journal of the American Chemical Society, 2020, 142, 16732-16747.	13.7	21
30	Counterion Dependence of Dinitrogen Activation and Functionalization by a Diniobium Hydride Anion. Angewandte Chemie, 2020, 132, 13546-13552.	2.0	1
31	The Reaction Pathway Leading to Dinuclear Rhodium and Iridium Complexes from Alkyne-Containing Bisphosphine Ligands. Bulletin of the Chemical Society of Japan, 2020, 93, 794-798.	3.2	4
32	Magnesiation of Aryl Fluorides Catalyzed by a Rhodiumâ€“Aluminum Complex. Journal of the American Chemical Society, 2020, 142, 11647-11652.	13.7	59
33	Structuralâ€Deformationâ€Energyâ€Modulation Strategy in a Soft Porous Coordination Polymer with an Interpenetrated Framework. Angewandte Chemie, 2020, 132, 15647-15651.	2.0	4
34	Structuralâ€Deformationâ€Energyâ€Modulation Strategy in a Soft Porous Coordination Polymer with an Interpenetrated Framework. Angewandte Chemie - International Edition, 2020, 59, 15517-15521.	13.8	38
35	Propene oxidation catalysis and electronic structure of M₅₅particles (M = Pd or Rh): differences and similarities between Pd₅₅and Rh₅₅. Physical Chemistry Chemical Physics, 2020, 22, 11783-11796.	2.8	5
36	Experimental and Theoretical Investigation of an S_N2-type Pathway for Borateâ€“Fluorine Bond Cleavage by Electron-Rich Late-Transition Metal Complexes. Inorganic Chemistry, 2020, 59, 4282-4291.	4.0	6

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37	Counterion Dependence of Dinitrogen Activation and Functionalization by a Diniobium Hydride Anion. Angewandte Chemie - International Edition, 2020, 59, 13444-13450.	13.8	12
38	Delocalization of the Excited State and Emission Spectrum of the Platinum(II) Bipyridine Complex in Crystal: Periodic QM/MM Study. Journal of Physical Chemistry C, 2020, 124, 10453-10461.	3.1	16
39	Evaluation of OHÂ·Â·Â·O Type Hydrogen Bond Energy in Native Cellulose by Quantum Chemical Calculations. Zairyo/Journal of the Society of Materials Science, Japan, 2020, 69, 459-464.	0.2	1
40	Pd/NHC-catalyzed cross-coupling reactions of nitroarenes. Chemical Communications, 2019, 55, 9291-9294.	4.1	41
41	Reaction Behavior of the NO Molecule on the Surface of an M_n Particle (M = Ru,) Tj ETQq1 1 0.784314 rgBT /Overlo Journal of Physical Chemistry A, 2019, 123, 7021-7033.	2.5	24
42	Development of dissociative force field for allâ€atomistic molecular dynamics calculation of fracture of polymers. Journal of Computational Chemistry, 2019, 40, 2571-2576.	3.3	5
43	Carbon dioxide capture and efficient fixation in a dynamic porous coordination polymer. Nature Communications, 2019, 10, 4362.	12.8	91
44	Reactions of a Silylyne Complex with Aldehydes: Formation of Wâ^'Siâ^'Oâ^'C Fourâ€Membered Metallacycles and Their Metathesisâ€Like Fragmentation. Chemistry - A European Journal, 2019, 25, 3795-3798.	3.3	11
45	Design and control of gas diffusion process in a nanoporous soft crystal. Science, 2019, 363, 387-391.	12.6	332
46	Dependence of Absorption and Emission Spectra on Polymorphs of Gold(I) Isocyanide Complexes: Theoretical Study with QM/MM Approach. Journal of Physical Chemistry C, 2019, 123, 4773-4794.	3.1	12
47	sp³ Câ€“H Borylation Catalyzed by Iridium(III) Triboryl Complex: Comprehensive Theoretical Study of Reactivity, Regioselectivity, and Prediction of Excellent Ligand. Journal of the American Chemical Society, 2019, 141, 9854-9866.	13.7	44
48	Heptacoordinate Structures of Organotin Halides with Three Phosphine Donors: Halogenâ€Substituent Effect on Geometry. European Journal of Inorganic Chemistry, 2019, 2019, 3045-3052.	2.0	2
49	Self-regeneration of a Niâ€“Cu alloy catalyst during a three-way catalytic reaction. Physical Chemistry Chemical Physics, 2019, 21, 18816-18822.	2.8	16
50	Theoretical prediction of Ni(I)â€catalyst for hydrosilylation of pyridine and quinoline. Journal of Computational Chemistry, 2019, 40, 2119-2130.	3.3	12
51	Characterization of Rhâ€“Al Bond in Rh(PAlP) (PAlP = Pincer-type Diphosphino-Aluminyl Ligand) in Comparison with Rh(L)(PMe₃)₂ (L = AlMe₂,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 18	4.0	27
52	Catalysis of Cu Cluster for NO Reduction by CO: Theoretical Insight into the Reaction Mechanism. ACS Omega, 2019, 4, 2596-2609.	3.5	36
53	How to understand very weak Crâ€“Cr double bonds and negative spin populations in trinuclear Cr complexes: theoretical insight. Physical Chemistry Chemical Physics, 2019, 21, 22976-22989.	2.8	3
54	Electronic processes in NO dimerization on Ag and Cu clusters: DFT and MRMP2 studies. Journal of Computational Chemistry, 2019, 40, 181-190.	3.3	9

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55	Theoretical Insight into Coreâ€“Shell Preference for Bimetallic Pt-M (M = Ru, Rh, Os, and Ir) Cluster and Its Electronic Structure. Journal of Physical Chemistry C, 2018, 122, 9081-9090.	3.1	15
56	Ni(I)-Hydride Catalyst for Hydrosilylation of Carbon Dioxide and Dihydrogen Generation: Theoretical Prediction and Exploration of Full Catalytic Cycle. Organometallics, 2018, 37, 1258-1270.	2.3	21
57	Theoretical Insight into Gate-Opening Adsorption Mechanism and Sigmoidal Adsorption Isotherm into Porous Coordination Polymer. Journal of the American Chemical Society, 2018, 140, 13958-13969.	13.7	48
58	Reversible Oxidative Addition/Reductive Elimination of a Siâ¯H Bond with Baseâ€Stabilized Silylenes: A Theoretical Insight. Chemistry - A European Journal, 2018, 24, 11377-11385.	3.3	7
59	Rhodium Complexes Bearing PAlP Pincer Ligands. Journal of the American Chemical Society, 2018, 140, 7070-7073.	13.7	96
60	Mechanism of NOâ€“CO reaction over highly dispersed cuprous oxide on Î³-alumina catalyst using a metalâ€“support interfacial site in the presence of oxygen: similarities to and differences from biological systems. Catalysis Science and Technology, 2018, 8, 3833-3845.	4.1	16
61	How To Perform Suzukiâ€“Miyaura Reactions of Nitroarene or Nitrations of Bromoarene Using a Pd⁰ Phosphine Complex: Theoretical Insight and Prediction. Organometallics, 2018, 37, 3480-3487.	2.3	24
62	QM/MM Approach to Isomerization of Ruthenium(II) Sulfur Dioxide Complex in Crystal; Comparison with Solution and Gas Phases. Journal of Physical Chemistry C, 2018, 122, 20701-20716.	3.1	5
63	Reversible Ï€-system switching of thiophene-fused thiahexaphyrins by solvent and oxidation/reduction. Chemical Science, 2018, 9, 7528-7539.	7.4	8
64	A Theoretical Investigation on CO Oxidation by Singleâ€Atom Catalysts M₁/Î³â€Al₂O₃ (M=Pd, Fe, Co, and Ni). ChemCatChem, 2017, 9, 1222-1229.	3.7	76
65	Reactions of Silanone(silyl)tungsten and -molybdenum Complexes with MesCNO, (Me₂SiO)₃, MeOH, and H₂O: Experimental and Theoretical Studies. Organometallics, 2017, 36, 1009-1018.	2.3	7
66	[2 + 2]-type Reaction of Metalâ€“Metal Ïƒ-Bond with Fullerene Forming an Î·1-C60 Metal Complex: Mechanistic Details of Formation Reaction and Prediction of a New Î·1-C60 Metal Complex. Inorganic Chemistry, 2017, 56, 6746-6754.	4.0	14
67	A coordination strategy to realize a sextuply-bonded complex. Physical Chemistry Chemical Physics, 2017, 19, 14947-14954.	2.8	8
68	Coreâ€“Shell versus Other Structures in Binary Cu₃₈â€“n</sub>M_n Nanoclusters (M = Ru, Rh, Pd, Ag, Os, Ir, Pt, and Au; n = 1, 2, and 6): Theoretical Insight into Determining Factors. Journal of Physical Chemistry C, 2017, 121, 10514-10528.	3.1	16
69	Iridium Hydride Mediated Stannaneâ€“Fluorine and â¯Chlorine Ïƒ-Bond Activation: Reversible Switching between X-Type Stannyl and Z-Type Stannane Ligands. Organometallics, 2017, 36, 2096-2106.	2.3	14
70	Theoretical study of one-electron-oxidized salen complexes of group 7 (Mn(<scp>iii</scp>),) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 152 T states in solution. Physical Chemistry Chemical Physics, 2017, 19, 16831-16849.	2.8	5
71	Photo absorption of â€coumaric acid in aqueous solution: RISMâ€SCFâ€SEDD theory approach. Journal of Computational Chemistry, 2017, 38, 1567-1573.	3.3	6
72	Moâ€“Mo Quintuple Bond is Highly Reactive in Hâ€“H, Câ€“H, and Oâ€“H Ïƒ-Bond Cleavages Because of the Polarized Electronic Structure in Transition State. Inorganic Chemistry, 2017, 56, 4011-4020.	4.0	20

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73	Structures of Bimetallic Copperâ€“Ruthenium Nanoparticles: Incoherent Interface and Surface Active Sites for Catalytic Nitric Oxide Dissociation. Journal of Physical Chemistry C, 2017, 121, 300-307.	3.1	15
74	Theoretical Study of Nickel-Catalyzed Selective Alkenylation of Pyridine: Reaction Mechanism and Crucial Roles of Lewis Acid and Ligands in Determining the Selectivity. Journal of Organic Chemistry, 2017, 82, 289-301.	3.2	34
75	How to Control Inversion vs Retention Transmetalation between Pd^{II}â€“Phenyl and Cu^Iâ€“Alkyl Complexes: Theoretical Insight. Journal of the American Chemical Society, 2017, 139, 14065-14076.	13.7	13
76	DFT Mechanistic Study on Alkene Hydrogenation Catalysis of Iron Metallaboratrane: Characteristic Features of Iron Species. Organometallics, 2017, 36, 3530-3538.	2.3	18
77	Embedded Cluster Model for Al₂O₃ and AlPO₄ Surfaces Using Point Charges and Periodic Electrostatic Potential. Journal of Physical Chemistry C, 2017, 121, 20242-20253.	3.1	7
78	Aromatic Câ€“H Ïƒ-Bond Activation by Ni⁰, Pd⁰, and Pt⁰ Alkene Complexes: Concerted Oxidative Addition to Metal vs Ligand-to-Ligand H Transfer Mechanism. Organometallics, 2017, 36, 2761-2771.	2.3	84
79	Density Gradation of Open Metal Sites in the Mesospace of Porous Coordination Polymers. Journal of the American Chemical Society, 2017, 139, 11576-11583.	13.7	118
80	Characteristic Features of CO₂ and CO Adsorptions to Paddle-Wheel-type Porous Coordination Polymer. Journal of Physical Chemistry C, 2017, 121, 19129-19139.	3.1	13
81	Cooperative Bond Scission in a Soft Porous Crystal Enables Discriminatory Gate Opening for Ethylene over Ethane. Journal of the American Chemical Society, 2017, 139, 18313-18321.	13.7	72
82	The Suzukiâ€“Miyaura Coupling of Nitroarenes. Journal of the American Chemical Society, 2017, 139, 9423-9426.	13.7	158
83	Transitionâ€Metalâ€Mediated Cleavage of Fluoroâ€Silanes under Mild Conditions. Chemistry - A European Journal, 2016, 22, 2370-2375.	3.3	30
84	Theoretical Study of Hydrogenation Catalysis of Phosphorus Compound and Prediction of Catalyst with High Activity and Wide Application Scope. ACS Catalysis, 2016, 6, 4859-4870.	11.2	26
85	Cooperative Catalysis of Combined Systems of Transitionâ€Metal Complexes with Lewis Acids: Theoretical Understanding. Chemical Record, 2016, 16, 2405-2425.	5.8	42
86	Catalytic Hydrogenation of Carbon Dioxide with Ammoniaâ€“Borane by Pincer-Type Phosphorus Compounds: Theoretical Prediction. Journal of the American Chemical Society, 2016, 138, 13481-13484.	13.7	41
87	Hetero-dinuclear complexes of 3d metals with a bridging dinitrogen ligand: theoretical prediction of the characteristic features of geometry and spin multiplicity. Physical Chemistry Chemical Physics, 2016, 18, 26365-26375.	2.8	3
88	para-Selective Alkylation of Benzamides and Aromatic Ketones by Cooperative Nickel/Aluminum Catalysis. Journal of the American Chemical Society, 2016, 138, 14699-14704.	13.7	149
89	Reductive Crossâ€Coupling of Conjugated Arylalkenes and Aryl Bromides with Hydrosilanes by Cooperative Palladium/Copper Catalysis. Angewandte Chemie - International Edition, 2016, 55, 6275-6279.	13.8	124
90	Optical control of neuronal firing via photoinduced electron transfer in donorâ€“acceptor conjugates. Chemical Science, 2016, 7, 3331-3337.	7.4	25

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91	3D-RISM-MP2 Approach to Hydration Structure of Pt(II) and Pd(II) Complexes: Unusual H-Ahead Mode vs Usual O-Ahead One. Journal of Chemical Theory and Computation, 2016, 12, 1189-1206.	5.3	13
92	Transition-Metal-Mediated Germaniumâ€“Fluorine Activation: Inverse Electron Flow in Ïƒ-Bond Metathesis. Organometallics, 2016, 35, 713-719.	2.3	34
93	Theoretical and Computational Study of a Complex System Consisting of Transition Metal Element(s): How to Understand and Predict Its Geometry, Bonding Nature, Molecular Property, and Reaction Behavior. Bulletin of the Chemical Society of Japan, 2015, 88, 889-938.	3.2	34
94	Activation of Strong Boronâ€“Fluorine and Siliconâ€“Fluorine Ïƒâ€Bonds: Theoretical Understanding and Prediction. Chemistry - A European Journal, 2015, 21, 13588-13597.	3.3	20
95	A DFT study of hydride transfers to the carbonyl oxygen of DDQ. International Journal of Quantum Chemistry, 2015, 115, 1533-1542.	2.0	11
96	How Can We Understand Au₈ Cores and Entangled Ligands of Selenolate- and Thiolate-Protected Gold Nanoclusters Au₂₄(ER)₂₀ and Au₂₀(ER)₁₆ (E = Se, S; R = Ph, Me)? A Theoretical Study. Journal of the American Chemical Society, 2015, 137, 8593-8602.	13.7	25
97	Evaluation of the Ïƒ-Donation from Group 11 Metals (Cu, Ag, Au) to Silane, Germane, and Stannane Based on the Experimental/Theoretical Systematic Approach. Organometallics, 2015, 34, 1440-1448.	2.3	46
98	Characterization of AlPO₄(110) Surface in Adsorption of Rh Dimer and Its Comparison with Î³-Al₂O₃(100) Surface: A Theoretical Study. Journal of Physical Chemistry C, 2015, 119, 19752-19762.	3.1	17
99	A molecular level study of selective cation capture by a hostâ€“guest mechanism for 25,26,27,28-tetramethoxycalix[4]arene in MClO₄solution (MÂ=ÂNa, K). Molecular Simulation, 2015, 41, 881-891.	2.0	1
100	Reasons Two Nonstrained Câ€“C Ïƒ-Bonds Can Be Easily Cleaved in Decyanative [4 + 2] Cycloaddition Catalyzed by Nickel(0)/Lewis Acid Systems. Theoretical Insight. ACS Catalysis, 2015, 5, 1-10.	11.2	55
101	Proton transfers in the Strecker reaction revealed by DFT calculations. Beilstein Journal of Organic Chemistry, 2014, 10, 1765-1774.	2.2	5
102	Substrate dependent reaction channels of the Wolffâ€“Kishner reduction reaction: A theoretical study. Beilstein Journal of Organic Chemistry, 2014, 10, 259-270.	2.2	11
103	Effects of PAr₃ Ligands on Direct Arylation of Heteroarenes with Isolated [Pd(2,6-Me₂C₆H₃)(Î¼-O₂CMe)(PAr₃)]₄ Complexes. Organometallics, 2014, 33, 6247-6252.	4.0	28
104	Interaction of Various Gas Molecules with Paddle-Wheel-Type Open Metal Sites of Porous Coordination Polymers: Theoretical Investigation. Inorganic Chemistry, 2014, 53, 2417-2426.	4.0	21
105	Self-Accelerating CO Sorption in a Soft Nanoporous Crystal. Science, 2014, 343, 167-170.	12.6	434
106	Synthesis, Geometry, and Bonding Nature of Heptacoordinate Compounds of Silicon and Germanium Featuring Three Phosphine Donors. Organometallics, 2014, 33, 6557-6567.	2.3	24
107	Can One Ïƒ*-Antibonding Orbital Interact with Six Electrons of Lewis Bases? Analysis of a Multiply Interacting Ïƒ* Orbital. Organometallics, 2014, 33, 5960-5963.	2.3	14
108	The important role of the Moâ€“Mo quintuple bond in catalytic synthesis of benzene from alkynes. A theoretical study. Dalton Transactions, 2014, 43, 11478-11492.	3.3	21

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109	Generation of Dihydrogen Molecule and Hydrosilylation of Carbon Dioxide Catalyzed by Zinc Hydride Complex: Theoretical Understanding and Prediction. Inorganic Chemistry, 2014, 53, 8485-8493.	4.0	43
110	The crucial roles of MgCl₂ as a non-innocent additive in the Ni-catalyzed carboxylation of benzyl halide with CO₂. Chemical Communications, 2014, 50, 13026-13029.	4.1	47
111	Theoretical Study of One-Electron Oxidized Mn(III)â€“ and Ni(II)â€“Salen Complexes: Localized vs Delocalized Ground and Excited States in Solution. Journal of Chemical Theory and Computation, 2014, 10, 1062-1073.	5.3	22
112	Ïƒ-Bond Activation of Small Molecules and Reactions Catalyzed by Transition-Metal Complexes: Theoretical Understanding of Electronic Processes. Inorganic Chemistry, 2014, 53, 6444-6457.	4.0	60
113	DRIFT and Theoretical Studies of Ethylene/Ethane Separation on Flexible and Microporous [Cu₂(2,3â€pyrazinedicarboxylate)₂(pyrazine)]_n. European Journal of Inorganic Chemistry, 2014, 2014, 2747-2752.	2.0	28
114	Theoretical Mechanistic Study of Novel Ni(0)-Catalyzed [6 â€“ 2 + 2] Cycloaddition Reactions of Isatoic Anhydrides with Alkynes: Origin of Facile Decarboxylation. Organometallics, 2013, 32, 7564-7574.	2.3	24
115	Factors Controlling the Reactivity of Heteroarenes in Direct Arylation with Arylpalladium Acetate Complexes. Organometallics, 2013, 32, 4423-4430.	2.3	47
116	The crucial role of a Ni(i) intermediate in Ni-catalyzed carboxylation of aryl chloride with CO2: a theoretical study. Chemical Communications, 2013, 49, 10715.	4.1	62
117	A theoretical study of luminescent vapochromic compounds including an AuCu2(NHC)2 core. Dalton Transactions, 2013, 42, 4809.	3.3	7
118	Unexpected Electronic Process of H₂ Activation by a New Nickel Borane Complex: Comparison with the Usual Homolytic and Heterolytic Activations. Inorganic Chemistry, 2013, 52, 2844-2853.	4.0	64
119	Absorption of CO₂ and CS₂ into the Hofmann-Type Porous Coordination Polymer: Electrostatic versus Dispersion Interactions. Journal of the American Chemical Society, 2013, 135, 4840-4849.	13.7	72
120	A 3D-RISM-SCF method with dual solvent boxes for a highly polarized system: application to 1,6-anhydrosugar formation reaction of phenyl Î±- and Î²-d-glucosides under basic conditions. Physical Chemistry Chemical Physics, 2013, 15, 6368.	2.8	11
121	Theoretical Study of Reactivity of Ge(II)-hydride Compound: Comparison with Rh(I)-Hydride Complex and Prediction of Full Catalytic Cycle by Ge(II)-hydride. Journal of the American Chemical Society, 2013, 135, 8955-8965.	13.7	41
122	Coronene-transition metal complex: View from quantum chemistry and statistical mechanics. , 2012, , .		0
123	Proposal of new QM/MM approach for geometry optimization of periodic molecular crystal: Self-consistent point charge representation for crystalline effect on target QM molecule. Chemical Physics Letters, 2012, 544, 77-82.	2.6	6
124	Oscillator Strength of Symmetry-Forbidden d-d Absorption of Octahedral Transition Metal Complex: Theoretical Evaluation. Inorganic Chemistry, 2012, 51, 2785-2792.	4.0	11
125	Evaluation Procedure of Electrostatic Potential in 3D-RISM-SCF Method and Its Application to Hydrolyses of Cis- and Transplatin Complexes. Journal of Physical Chemistry B, 2012, 116, 13045-13062.	2.6	27
126	A Theoretical Study of an Unusual Y-Shaped Three-Coordinate Pt Complex: Pt(0) Ïƒ-Disilane Complex or Pt(II) Disilyl Complex?. Journal of the American Chemical Society, 2012, 134, 11749-11759.	13.7	36

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127	Systematic assessment on aqueous pK_a and pK_b of an amino acid base on RISMâ€SCFâ€SEDD method: Toward first principles calculations. International Journal of Quantum Chemistry, 2012, 112, 103-112.	2.0	6
128	Twoâ€step evaluation of binding energy and potential energy surface of van der Waals complexes. Journal of Computational Chemistry, 2012, 33, 617-628.	3.3	18
129	Theoretical Study of Ïƒ-Bond Activation Reactions and Catalytic Reactions by Transition Metal Complexes. , 2012, , 391-434.		7
130	Theoretical Study of Pt(PR₃)₂(AlCl₃) (R = H, Me, Ph, or Cy) Including an Unsupported Bond between Transition Metal and Non-transition Metal Elements: Geometry, Bond Strength, and Prediction. Journal of Physical Chemistry A, 2011, 115, 8520-8527.	2.5	9
131	Noble Reaction Features of Bromoborane in Oxidative Addition of Bâ€“Br Ïƒ-Bond to [M(PMe₃)₂] (M = Pt or Pd): Theoretical Study. Inorganic Chemistry, 2011, 50, 5290-5297.	4.0	29
132	Theoretical study of metallasilatranes; Bonding nature and prediction of new metallasilatrane. Collection of Czechoslovak Chemical Communications, 2011, 76, 619-629.	1.0	8
133	Theoretical study on high-spin to low-spin transition of {Fe(pyrazine)[Pt(CN)4]}: Guest-induced entropy decrease. Chemical Physics Letters, 2011, 511, 399-404.	2.6	24
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