Shigeyoshi Sakaki

List of Publications by Year
in descending order

187 papers	7,109 citations	58072 44 h-index	72025 76 g-index
193 all docs	193 docs citations	193 times ranked	6591 citing authors

#	Article	IF	Citations
1	Bidirectional Chemoâ€Switching of Spin State in a Microporous Framework. Angewandte Chemie - International Edition, 2009, 48, 4767-4771.	14.2	474
2	Self-Accelerating CO Sorption in a Soft Nanoporous Crystal. Science, 2014, 343, 167-170.	12.8	434
3	Design and control of gas diffusion process in a nanoporous soft crystal. Science, 2019, 363, 387-391.	12.8	332
4	Iridium-Catalyzed Borylation of Benzene with Diboron. Theoretical Elucidation of Catalytic Cycle Including Unusual Iridium(V) Intermediate. Journal of the American Chemical Society, 2003, 125, 16114-16126.	14.2	266
5	Câˆ'H Bond Activation of Benzene and Methane by M(Î·2-O2CH)2 (M = Pd or Pt). A Theoretical Study. Organometallics, 2000, 19, 3895-3908.	2.5	205
6	The Suzukiâ€"Miyaura Coupling of Nitroarenes. Journal of the American Chemical Society, 2017, 139, 9423-9426.	14.2	158
7	Theoretical Study of Trans-metalation Process in Palladium-Catalyzed Borylation of Iodobenzene with Diboron. Journal of the American Chemical Society, 2004, 126, 10457-10471.	14.2	153
8	para-Selective Alkylation of Benzamides and Aromatic Ketones by Cooperative Nickel/Aluminum Catalysis. Journal of the American Chemical Society, 2016, 138, 14699-14704.	14.2	149
9	Reductive Crossâ€Coupling of Conjugated Arylalkenes and Aryl Bromides with Hydrosilanes by Cooperative Palladium/Copper Catalysis. Angewandte Chemie - International Edition, 2016, 55, 6275-6279.	14.2	124
10	A Dualâ€Ligand Porous Coordination Polymer Chemiresistor with Modulated Conductivity and Porosity. Angewandte Chemie - International Edition, 2020, 59, 172-176.	14.2	124
11	Oxidative addition reactions of saturated Si-X bonds (X = H, F, C, or Si) to Pt(PH3)2. An ab initio MO/MP4 study. Journal of the American Chemical Society, 1993, 115, 2373-2381.	14.2	120
12	Density Gradation of Open Metal Sites in the Mesospace of Porous Coordination Polymers. Journal of the American Chemical Society, 2017, 139, 11576-11583.	14.2	118
13	Hostâ€"Guest Interaction Modulation in Porous Coordination Polymers for Inverse Selective CO₂/C₂H₂Separation. Angewandte Chemie - International Edition, 2021, 60, 11688-11694.	14.2	115
14	Theoretical Study of the Cp2Zr-Catalyzed Hydrosilylation of Ethylene. Reaction Mechanism Including New Ïƒ-Bond Activation. Journal of the American Chemical Society, 2004, 126, 3332-3348.	14.2	105
15	Rhodium Complexes Bearing PAlP Pincer Ligands. Journal of the American Chemical Society, 2018, 140, 7070-7073.	14.2	96
16	Theoretical Study on Ïƒ-Bond Activation of (HO)2Bâˆ'XH3by M(PH3)2(X = C, Si, Ge, or Sn; M = Pd or Pt). Noteworthy Contribution of the Boryl pÏ€Orbital to Mâˆ'Boryl Bonding and Activation of the Bâˆ'X Ïƒ-Bond. Organometallics, 1999, 18, 4825-4837.	2.5	93
17	Carbon dioxide capture and efficient fixation in a dynamic porous coordination polymer. Nature Communications, 2019, 10, 4362.	13.0	91
18	Why Does Fluoride Anion Accelerate Transmetalation between Vinylsilane and Palladium(II)âˆ'Vinyl Complex? Theoretical Study. Journal of the American Chemical Society, 2008, 130, 12975-12985.	14.2	88

#	Article	IF	Citations
19	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.	2.5	84
20	Is a Transition State Planar or Nonplanar in Oxidative Additions of Câˆ’H, Siâˆ’H, Câˆ’C, and Siâˆ’C Ïƒ-Bonds to Pt(PH3)2? A Theoretical Study. Journal of Physical Chemistry A, 1998, 102, 8027-8036.	2.5	78
21	Reaction of BX2âˆ’BX2(X = H or OH) with M(PH3)2(M = Pd or Pt). A Theoretical Study of the Characteristic Features. Inorganic Chemistry, 1997, 36, 226-229.	4.2	76
22	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
23	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.	14.2	72
24	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.	14.2	72
25	Theoretical Study of Câˆ’H and Nâˆ’H Ïƒ-Bond Activation Reactions by Titinium(IV)-Imido Complex. Good Understanding Based on Orbital Interaction and Theoretical Proposal for Nâˆ’H Ïƒ-Bond Activation of Ammonia. Journal of the American Chemical Society, 2007, 129, 8615-8624.	14.2	65
26	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.	4.2	64
27	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.	4.2	62
28	Tunable acetylene sorption by flexible catenated metalâ€“organic frameworks. Nature Chemistry, 2022, 14, 816-822.	14.2	62
29	A Theoretical Study of Nickel(0)-Catalyzed Phenylcyanation of Alkynes. Reaction Mechanism and Regioselectivity. Organometallics, 2009, 28, 2583-2594.	2.5	60
30	Ïƒ-Bond Activation of Small Molecules and Reactions Catalyzed by Transition-Metal Complexes: Theoretical Understanding of Electronic Processes. Inorganic Chemistry, 2014, 53, 6444-6457.	4.2	60
31	Magnesiation of Aryl Fluorides Catalyzed by a Rhodiumâ€“Aluminum Complex. Journal of the American Chemical Society, 2020, 142, 11647-11652.	14.2	59
32	A Theoretical Study of the Câˆ’H Activation of Methane Derivatives. Significant Effects of Electron-Withdrawing Substituents. Organometallics, 1998, 17, 1278-1289.	2.5	58
33	Theoretical Study of M(PH3)2Complexes of C60, Corannulene (C20H10), and Sumanene (C21H12) (M = Pd) Tj ETQq1 1 0.784314 rg BT 8055-8063.	2.5	56
34	Pd(ii)-promoted direct cross-coupling reaction of arenes via highly regioselective aromatic Câ€“H activation: a theoretical study. Dalton Transactions, 2010, 39, 3279.	3.3	55
35	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.	11.4	55
36	Comparison of Electronic Structure Theories for Solvated Molecules:â€‰ RISM-SCF versus PCM. Journal of Physical Chemistry A, 2004, 108, 1629-1634.	2.5	53

#	Article	IF	Citations
37	Ab initio MO study of carbon dioxide insertion into a copper(I)-hydrogen bond. Semiquantitative understanding of changes in geometry, bonding, and electron distribution during the reaction. Inorganic Chemistry, 1989, 28, 2583-2590.	4.2	51
38	Theoretical Study of Pyrazolate-Bridged Dinuclear Platinum(II) Complexes: Interesting Potential Energy Curve of the Lowest Energy Triplet Excited State and Phosphorescence Spectra. Inorganic Chemistry, 2008, 47, 4329-4337.	4.2	51
39	Theoretical Study of the Structure, Bonding Nature, and Reductive Elimination Reaction of Pd(XH3)(Î·3-C3H5)(PH3) (X = C, Si, Ge, Sn). Hypervalent Behavior of Group 14 Elements. Organometallics, 1999, 18, 4015-4026.	2.5	50
40	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.	14.2	48
41	Factors Controlling the Reactivity of Heteroarenes in Direct Arylation with Arylpalladium Acetate Complexes. Organometallics, 2013, 32, 4423-4430.	2.5	47
42	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.	4.2	47
43	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.	2.5	46
44	Bonding nature and reaction behavior of inter-element linkages with transition metal complexes. A theoretical study. Journal of Organometallic Chemistry, 2000, 611, 288-298.	1.9	45
45	Ab Initio MO Study of the CO2 Insertion into the Cu(I)-R Bond (R = H, CH3, or OH). Comparison between the CO2 Insertion and the C2H4 Insertion. Inorganic Chemistry, 1995, 34, 1914-1923.	4.2	44
46	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.	14.2	44
47	Geometries, Bonding Nature, and Relative Stabilities of Dinuclear Palladium(I) Ï€-Allyl and Mononuclear Palladium(II) Ï€-Allyl Complexes. A Theoretical Study. Organometallics, 1997, 16, 2995-3003.	2.5	43
48	Generation of Dihydrogen Molecule and Hydrosilylation of Carbon Dioxide Catalyzed by Zinc Hydride Complex: Theoretical Understanding and Prediction. Inorganic Chemistry, 2014, 53, 8485-8493.	4.2	43
49	Theoretical Study of Rhenium Dinuclear Complexes:Â Reâ‹¯Re Bonding Nature and Electronic Structure. Journal of Physical Chemistry A, 2006, 110, 9710-9717.	2.5	42
50	Cooperative Catalysis of Combined Systems of Transitionâ€Metal Complexes with Lewis Acids: Theoretical Understanding. Chemical Record, 2016, 16, 2405-2425.	5.9	42
51	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.	14.2	41
52	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.	14.2	41
53	Pd/NHC-catalyzed cross-coupling reactions of nitroarenes. Chemical Communications, 2019, 55, 9291-9294.	4.2	41
54	Oxidative addition of silane to Pt(PH3)2. An ab initio MO/MP4 study. Journal of the American Chemical Society, 1991, 113, 5063-5065.	14.2	40

#	Article	IF	Citations
55	Structuralâ€Deformationâ€Energyâ€Modulation Strategy in a Soft Porous Coordination Polymer with an Interpenetrated Framework. Angewandte Chemie - International Edition, 2020, 59, 15517-15521.	14.2	38
56	Oxygen Atom Transfer Reactions of Iridium and Osmium Complexes: Theoretical Study of Characteristic Features and Significantly Large Differences Between These Two Complexes. Inorganic Chemistry, 2009, 48, 8154-8163.	4.2	37
57	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.	14.2	36
58	Catalysis of Cu Cluster for NO Reduction by CO: Theoretical Insight into the Reaction Mechanism. ACS Omega, 2019, 4, 2596-2609.	3.6	36
59	Solvation effects in oxidative addition reaction of Methyliodide to Pt(II) complex: A theoretical study with RISMâ€“SCF method. Chemical Physics Letters, 2008, 458, 329-332.	2.6	35
60	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.	3.3	34
61	Transition-Metal-Mediated Germaniumâ€“Fluorine Activation: Inverse Electron Flow in Ïƒ-Bond Metathesis. Organometallics, 2016, 35, 713-719.	2.5	34
62	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.	3.3	34
63	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.	14.2	33
64	Theoretical and computational studies of organometallic reactions: successful or not?. Chemical Record, 2010, 10, 29-45.	5.9	31
65	Transitionâ€Metalâ€Mediated Cleavage of Fluoroâ€Silanes under Mild Conditions. Chemistry - A European Journal, 2016, 22, 2370-2375.	3.4	30
66	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.	4.2	29
67	Effects of PAr₃ Ligands on Direct Arylation of Heteroarenes with Isolated [Pd(2,6-Me₂C₆H₃)(Î¼-O₂CMe)(PAr₃)]₂ Complexes. Organometallics, 2014, 33, 6247-6252.	2.5	28
68	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.	2.1	28
69	Modulating fluorescence of 8-quinolinolato compounds by functional groups: A theoretical study. Applied Physics Letters, 2001, 79, 2348-2350.	3.4	27
70	Theoretical Study of Oxidative Additions of H₂ and MeCN to a Nickel(0) Complex:â€‰ Significantly Large Correlation Effects and Characteristic Features of the Reaction. Journal of Physical Chemistry A, 2007, 111, 7915-7924.	2.5	27
71	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.	2.7	27
72	Characterization of Rhâ€“Al Bond in Rh(PAlP) (PAlP = Pincer-type Diphosphino-Aluminyl Ligand) in Comparison with Rh(L)(PMe₃)₂ (L = AlMe₂,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 62 Td (Al(NM	4.2	27

#	Article	IF	Citations
73	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.	11.4	26
74	How to Stabilize Î·³-Silapropargyl/Alkynylsilyl Complex of [CpL₂M]⁺(L = CO, PMe₃, or PF₃ and M =) Tj ETQq0 0 0 rgBT /Overlo	2.5	25
75	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.	14.2	25
76	Optical control of neuronal firing via photoinduced electron transfer in donorâ€“acceptor conjugates. Chemical Science, 2016, 7, 3331-3337.	7.6	25
77	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
78	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.	2.5	24
79	Synthesis, Geometry, and Bonding Nature of Heptacoordinate Compounds of Silicon and Germanium Featuring Three Phosphine Donors. Organometallics, 2014, 33, 6557-6567.	2.5	24
80	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.	2.5	24
81	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
82	Insertion of carbon dioxide into a rhodium(III)â€“hydride bond: a theoretical studyâ€Šâ€. Journal of the Chemical Society Dalton Transactions, 1998, , 577-584.	1.1	23
83	Theoretical Study of Tungsten Î·³-Silaallyl/Î·³-Vinylsilyl and Vinyl Silylene Complexes:â€‰ Interesting Bonding Nature and Relative Stability. Organometallics, 2007, 26, 4413-4423.	2.5	23
84	Experimental and Theoretical Study of a Tungsten Dihydride Silyl Complex: New Insight into Its Bonding Nature and Fluxional Behavior. Organometallics, 2010, 29, 6267-6281.	2.5	23
85	Binding energies and bonding nature of MX(CO)(PH3)2(C60) (M=Rh or Ir; X=H or Cl): Theoretical study. Journal of Organometallic Chemistry, 2007, 692, 299-306.	1.9	22
86	Synthesis, Structure, and Bonding Nature of Ethynediyl-Bridged Bis(silylene) Dinuclear Complexes of Tungsten and Molybdenum. Organometallics, 2011, 30, 4515-4531.	2.5	22
87	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.	5.4	22
88	An ab initio molecular-orbital study of insertion of CO2into a RhIâ€“H bond. Journal of the Chemical Society Dalton Transactions, 1994, , 3047-3054.	1.1	21
89	Interaction of Various Gas Molecules with Paddle-Wheel-Type Open Metal Sites of Porous Coordination Polymers: Theoretical Investigation. Inorganic Chemistry, 2014, 53, 2417-2426.	4.2	21
90	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

#	Article	IF	Citations
91	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.	2.5	21
92	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.	14.2	21
93	Activation of Strong Boronâ€“Fluorine and Siliconâ€“Fluorine Ïƒâ€Bonds: Theoretical Understanding and Prediction. Chemistry - A European Journal, 2015, 21, 13588-13597.	3.4	20
94	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.	4.2	20
95	Aurophilicityâ€Mediated Construction of Emissive Porous Molecular Crystals as Versatile Hosts for Liquid and Solid Guests. Chemistry - A European Journal, 2020, 26, 735-744.	3.4	19
96	C2-selective alkylation of pyridines by rhodiumâ€“aluminum complexes. Tetrahedron, 2021, 95, 132339.	2.0	19
97	Twoâ€step evaluation of binding energy and potential energy surface of van der Waals complexes. Journal of Computational Chemistry, 2012, 33, 617-628.	3.4	18
98	DFT Mechanistic Study on Alkene Hydrogenation Catalysis of Iron Metallaboratrane: Characteristic Features of Iron Species. Organometallics, 2017, 36, 3530-3538.	2.5	18
99	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.	9.2	18
100	Hostâ€“Guest Interaction Modulation in Porous Coordination Polymers for Inverse Selective CO₂/C₂H₂Separation. Angewandte Chemie, 2021, 133, 11794-11800.	2.0	18
101	{2 + 2} Cycloaddition of Alkyne with Titaniumâ‹Imido Complex: Theoretical Study of Determining Factor of Reactivity and Regioselectivity. Journal of Physical Chemistry A, 2010, 114, 659-665.	2.5	17
102	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.	3.2	17
103	Acetylene-insertion reactions into Pt(II)-H and Pt(II)-SiH 3 bonds. An ab initio MO study and analysis based on the vibronic coupling model. Theoretical Chemistry Accounts, 1999, 102, 377-384.	1.4	16
104	Coreâ€“Shell versus Other Structures in Binary Cu_{38â€“n}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.	3.2	16
105	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.	4.2	16
106	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
107	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.	3.2	16
108	Bonding Nature of Open-Lantern-type Dinuclear Cr(II) Complexes. Theoretical Study with the MRMP2 Method. Journal of Physical Chemistry A, 2009, 113, 3202-3209.	2.5	15

#	Article	IF	Citations
109	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.	3.2	15
110	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.	3.2	15
111	Can One Ïƒ*-Antibonding Orbital Interact with Six Electrons of Lewis Bases? Analysis of a Multiply Interacting Ïƒ* Orbital. Organometallics, 2014, 33, 5960-5963.	2.5	14
112	[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.	4.2	14
113	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.	2.5	14
114	Control of local flexibility towards p-xylene sieving in Hofmann-type porous coordination polymers. Chemical Communications, 2020, 56, 9632-9635.	4.2	14
115	Significant differences in electronic structure among X-, Î±- and Î²-forms of lithium phthalocyanine. Dalton Transactions, 2003, , 31-33.	3.3	13
116	Solvation effect on the interaction between sodium and chloride ions in aqueous solution: An analysis based on the new resonance theory. International Journal of Quantum Chemistry, 2007, 107, 3132-3136.	2.0	13
117	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.	5.4	13
118	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.	14.2	13
119	Characteristic Features of CO₂ and CO Adsorptions to Paddle-Wheel-type Porous Coordination Polymer. Journal of Physical Chemistry C, 2017, 121, 19129-19139.	3.2	13
120	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.	6.4	13
121	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.	3.2	12
122	Theoretical prediction of Ni(I)â€catalyst for hydrosilylation of pyridine and quinoline. Journal of Computational Chemistry, 2019, 40, 2119-2130.	3.4	12
123	Counterion Dependence of Dinitrogen Activation and Functionalization by a Diniobium Hydride Anion. Angewandte Chemie - International Edition, 2020, 59, 13444-13450.	14.2	12
124	A theoretical study on CO2 insertion into an M(bond)H bond (M = Rh and Cu). International Journal of Quantum Chemistry, 1996, 57, 481-491.	2.0	11
125	Binding energy of gas molecule with two pyrazine molecules as organic linker in metalâ€“organic framework: its theoretical evaluation and understanding of determining factors. Theoretical Chemistry Accounts, 2011, 130, 475-482.	1.4	11
126	Oscillator Strength of Symmetry-Forbidden d-d Absorption of Octahedral Transition Metal Complex: Theoretical Evaluation. Inorganic Chemistry, 2012, 51, 2785-2792.	4.2	11

#	Article	IF	Citations
127	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
128	Substrate dependent reaction channels of the Wolffâ€“Kishner reduction reaction: A theoretical study. Beilstein Journal of Organic Chemistry, 2014, 10, 259-270.	2.3	11
129	A DFT study of hydride transfers to the carbonyl oxygen of DDQ. International Journal of Quantum Chemistry, 2015, 115, 1533-1542.	2.0	11
130	Reactions of a Silylyne Complex with Aldehydes: Formation of Wâˆ’Siâˆ’Oâˆ’C Fourâ€Membered Metallacycles and Their Metathesisâ€Like Fragmentation. Chemistry - A European Journal, 2019, 25, 3795-3798.	3.4	11
131	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.	6.4	11
132	Methylviologen-pendant iron porphyrins as models of a reduction enzyme: six-electron reduction of nitrobenzene to anilineElectronic supplementary information (ESI) available: time-courses of reduction, UV-VIS spectral changes, cyclic voltammograms, EPR spectra, conversion and yield percentages for the reduction of p-nitroanisole. See http://www.rsc.org/suppdata/dt/b2/b211125j/. Dalton Transactions, 2003, , 1153-1160.	3.3	10
133	Generalization of the New Resonance Theory: Second Quantization Operator, Localization Scheme, and Basis Set. Journal of Chemical Theory and Computation, 2009, 5, 1741-1748.	5.4	10
134	Inverted-sandwich-type and open-lantern-type dinuclear transition metal complexes: theoretical study of chemical bonds by electronic stress tensor. Theoretical Chemistry Accounts, 2011, 130, 237-250.	1.4	10
135	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.	3.3	10
136	Kinetic study of the photo-induced electron transfer reaction between ruthenium(ii) complexes of 2,2â€²-bipyridine derivatives and methyl viologen. Effects of bulky substituents introduced onto 2,2â€²-bipyridine. Dalton Transactions, 2003, , 692-698.	3.3	9
137	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
138	Electronic processes in NO dimerization on Ag and Cu clusters: DFT and MRMP2 studies. Journal of Computational Chemistry, 2019, 40, 181-190.	3.4	9
139	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.	4.2	9
140	Can Cp2Zr(C2H4) Easily React with Hydrosilane? Theoretical Study. Chemistry Letters, 2001, 30, 1222-1223.	1.4	8
141	Theoretical study of metallasilatranes; Bonding nature and prediction of new metallasilatrane. Collection of Czechoslovak Chemical Communications, 2011, 76, 619-629.	1.0	8
142	A coordination strategy to realize a sextuply-bonded complex. Physical Chemistry Chemical Physics, 2017, 19, 14947-14954.	2.8	8
143	Reversible Ï€-system switching of thiophene-fused thiahexaphyrins by solvent and oxidation/reduction. Chemical Science, 2018, 9, 7528-7539.	7.6	8
144	A Dualâ€Ligand Porous Coordination Polymer Chemiresistor with Modulated Conductivity and Porosity. Angewandte Chemie, 2020, 132, 178-182.	2.0	8

#	Article	IF	Citations
145	Efficient reduction catalysis of viologen-bound iron porphyrin and its application to six-electron reduction of nitrobenzene to anilineâ€Šâ€. Dalton Transactions RSC, 2000, , 1015-1017.	2.3	7
146	Novel photo-induced deracemization of [Co(acac)3] (acacâ€…=â€…acetylacetonate) with a chiral ruthenium(II) complex, Î”-[Ru(menbpy)3]2+ (menbpyâ€…=â€…4,4â€²-bis{(1R,2S,5R)-(âˆ’)-menthoxycarbonyl}-2,2â€²-bipyridine). Reaction mechanism and significant effects of solvent and anionâ€Šâ€. Dalton Transactions RSC, 2001, , 928-934.	2.3	7
147	A theoretical study of luminescent vapochromic compounds including an AuCu2(NHC)2 core. Dalton Transactions, 2013, 42, 4809.	3.3	7
148	Reactions of Silanone(silyl)tungsten and -molybdenum Complexes with MesCNO, (Me₂SiO)₃, MeOH, and H₂O: Experimental and Theoretical Studies. Organometallics, 2017, 36, 1009-1018.	2.5	7
149	Embedded Cluster Model for Al₂O₃ and AlPO₄ Surfaces Using Point Charges and Periodic Electrostatic Potential. Journal of Physical Chemistry C, 2017, 121, 20242-20253.	3.2	7
150	Reversible Oxidative Addition/Reductive Elimination of a Siâˆ’H Bond with Baseâ€Stabilized Silylenes: A Theoretical Insight. Chemistry - A European Journal, 2018, 24, 11377-11385.	3.4	7
151	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.	2.9	7
152	Theoretical Study of Ïƒ-Bond Activation Reactions and Catalytic Reactions by Transition Metal Complexes. , 2012, , 391-434.		7
153	Theoretical Study on Siâˆ’Cl Bond Activation in Pdâ€Catalyzed Crossâ€Coupling of Chlorosilanes with Organoaluminum. European Journal of Organic Chemistry, 2022, 2022, .	2.4	7
154	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
155	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
156	Photo absorption of â€coumaric acid in aqueous solution: RISMâ€SCFâ€SEDD theory approach. Journal of Computational Chemistry, 2017, 38, 1567-1573.	3.4	6
157	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.	4.2	6
158	Proton transfers in the Strecker reaction revealed by DFT calculations. Beilstein Journal of Organic Chemistry, 2014, 10, 1765-1774.	2.3	5
159	Theoretical study of one-electron-oxidized salen complexes of group 7 (Mn(<scp>iii</scp>),) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf states in solution. Physical Chemistry Chemical Physics, 2017, 19, 16831-16849.	2.8	5
160	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.	3.2	5
161	Development of dissociative force field for allâ€atomistic molecular dynamics calculation of fracture of polymers. Journal of Computational Chemistry, 2019, 40, 2571-2576.	3.4	5
162	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

#	Article	IF	Citations
163	Theoretical Study of NO Dissociative Adsorption onto 3d Metal Particles M₅₅ (M = Fe, Co,) Tj ETQq1 1 0.784314 rgBT /Ov ACS Omega, 2021, 6, 4888-4898.	3.6	5
164	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.	11.4	5
165	Molecule in soft-crystal at ground and excited states: Theoretical approach. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2022, 51, 100482.	11.9	5
166	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.	11.4	5
167	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.	3.3	4
168	Structuralâ€Deformationâ€Energyâ€Modulation Strategy in a Soft Porous Coordination Polymer with an Interpenetrated Framework. Angewandte Chemie, 2020, 132, 15647-15651.	2.0	4
169	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
170	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
171	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
172	O₂activation by coreâ€“shell Ru₁₃@Pt₄₂particles in comparison with Pt₅₅particles: a DFT study. RSC Advances, 2020, 10, 36090-36100.	3.7	3
173	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.	3.2	3
174	Heptacoordinate Structures of Organotin Halides with Three Phosphine Donors: Halogenâ€Substituent Effect on Geometry. European Journal of Inorganic Chemistry, 2019, 2019, 3045-3052.	2.1	2
175	Deacylative Carbonâ€Carbon Bond Cleavage of Ketone Equivalents: Applications to Radical Carbonâ€Carbon Bond Formation Reactions. Chemistry - an Asian Journal, 2021, 16, 282-286.	3.4	2
176	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.	4.2	2
177	Reply to â€œComment on â€˜Analysis on Solvated Molecules with a New Energy Partitioning Scheme for Intra- and Intermolecular Interactions'â€. Journal of Physical Chemistry B, 2007, 111, 672-674.	2.7	1
178	Theoretical investigation of Î¼â€Oâ€bridged dinuclear Re complexes: Electronic structure, bonding nature, and absorption spectra. International Journal of Quantum Chemistry, 2009, 109, 2319-2327.	2.0	1
179	A Festschrift in honor of Shigeru Nagase. Theoretical Chemistry Accounts, 2011, 130, 129-152.	1.4	1
180	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.	1.9	1

#	Article	IF	Citations
181	Counterion Dependence of Dinitrogen Activation and Functionalization by a Diniobium Hydride Anion. Angewandte Chemie, 2020, 132, 13546-13552.	2.0	1
182	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.	4.2	1
183	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
184	.SIGMA.-Bond Activation by Transition Metal Complexes and Its Analogous Reactions. A Theoretical Study.. Yuki Gosei Kagaku Kyokaishi/Journal of Synthetic Organic Chemistry, 2000, 58, 1189-1201.	0.1	1
185	Coronene-transition metal complex: View from quantum chemistry and statistical mechanics. , 2012, , .		0
186	Frontispiz: Hostâ€“Guest Interaction Modulation in Porous Coordination Polymers for Inverse Selective CO₂/C₂H₂ Separation. Angewandte Chemie, 2021, 133, .	2.0	0
187	Frontispiece: Hostâ€“Guest Interaction Modulation in Porous Coordination Polymers for Inverse Selective CO₂/C₂H₂ Separation. Angewandte Chemie - International Edition, 2021, 60, .	14.2	0