Shigeyoshi Sakaki Or S Sakaki

List of Publications by Year
in descending order

226 papers	10,324 citations	31976 53 h-index	49909 87 g-index
231 all docs	231 docs citations	231 times ranked	8380 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	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
7	Theoretical Study of NO Dissociative Adsorption onto 3d Metal Particles M₅₅ (M = Fe, Co,) Tj ETQq1 1 0.784314 rgBT /O ACS Omega, 2021, 6, 4888-4898.	3.5	5
8	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
9	Heterometallic d⁸–d¹⁰ Coupling of Rh(I) and M(0) (M=Pd, Pt) in a Sandwich Framework of Ï€â€Conjugated Ligands. Chemistry - A European Journal, 2021, 27, 10558-10562.	3.3	0
10	Pincerâ€Type Phosphorus Compounds With Borylâ€Pendant And Application In Catalytic H 2 Generation From Ammoniaâ€Borane: A Theoretical Study. ChemCatChem, 2021, 13, 3925-3929.	3.7	3
11	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
12	C2-selective alkylation of pyridines by rhodiumâ€“aluminum complexes. Tetrahedron, 2021, 95, 132339.	1.9	19
13	A Dualâ€Ligand Porous Coordination Polymer Chemiresistor with Modulated Conductivity and Porosity. Angewandte Chemie - International Edition, 2020, 59, 172-176.	13.8	124
14	A Dualâ€Ligand Porous Coordination Polymer Chemiresistor with Modulated Conductivity and Porosity. Angewandte Chemie, 2020, 132, 178-182.	2.0	8
15	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
16	O₂activation by coreâ€“shell Ru₁₃@Pt₄₂particles in comparison with Pt₅₅particles: a DFT study. RSC Advances, 2020, 10, 36090-36100.	3.6	3
17	Control of local flexibility towards p-xylene sieving in Hofmann-type porous coordination polymers. Chemical Communications, 2020, 56, 9632-9635.	4.1	14
18	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

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19	Magnesiation of Aryl Fluorides Catalyzed by a Rhodiumâ€“Aluminum Complex. Journal of the American Chemical Society, 2020, 142, 11647-11652.	13.7	59
20	Structuralâ€Deformationâ€Energyâ€Modulation Strategy in a Soft Porous Coordination Polymer with an Interpenetrated Framework. Angewandte Chemie, 2020, 132, 15647-15651.	2.0	4
21	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
22	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
23	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
24	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
25	Pd/NHC-catalyzed cross-coupling reactions of nitroarenes. Chemical Communications, 2019, 55, 9291-9294.	4.1	41
26	Reaction Behavior of the NO Molecule on the Surface of an M_n Particle (M = Ru,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Journal of Physical Chemistry A, 2019, 123, 7021-7033.	2.5	24
27	Carbon dioxide capture and efficient fixation in a dynamic porous coordination polymer. Nature Communications, 2019, 10, 4362.	12.8	91
28	Design and control of gas diffusion process in a nanoporous soft crystal. Science, 2019, 363, 387-391.	12.6	332
29	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
30	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
31	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
32	Theoretical prediction of Ni(I)â€catalyst for hydrosilylation of pyridine and quinoline. Journal of Computational Chemistry, 2019, 40, 2119-2130.	3.3	12
33	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
34	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
35	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
36	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

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37	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
38	Rhodium Complexes Bearing PAlP Pincer Ligands. Journal of the American Chemical Society, 2018, 140, 7070-7073.	13.7	96
39	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
40	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
41	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
42	[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
43	A coordination strategy to realize a sextuply-bonded complex. Physical Chemistry Chemical Physics, 2017, 19, 14947-14954.	2.8	8
44	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
45	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
46	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
47	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
48	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
49	DFT Mechanistic Study on Alkene Hydrogenation Catalysis of Iron Metallaboratrane: Characteristic Features of Iron Species. Organometallics, 2017, 36, 3530-3538.	2.3	18
50	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
51	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
52	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
53	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
54	The Suzukiâ€“Miyaura Coupling of Nitroarenes. Journal of the American Chemical Society, 2017, 139, 9423-9426.	13.7	158

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55	Transitionâ€Metalâ€Mediated Cleavage of Fluoroâ€Silanes under Mild Conditions. Chemistry - A European Journal, 2016, 22, 2370-2375.	3.3	30
56	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
57	Cooperative Catalysis of Combined Systems of Transitionâ€Metal Complexes with Lewis Acids: Theoretical Understanding. Chemical Record, 2016, 16, 2405-2425.	5.8	42
58	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
59	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
60	Theoretical Study of Pd₁₁Si₆ Nanosheet Compounds Including Sevenâ€Coordinated Si Species and Its Ge Analogues. Chemistry - A European Journal, 2016, 22, 1076-1087.	3.3	13
61	Transition-Metal-Mediated Germaniumâ€“Fluorine Activation: Inverse Electron Flow in Ïƒ-Bond Metathesis. Organometallics, 2016, 35, 713-719.	2.3	34
62	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
63	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
64	Heterolytic Activation of Dihydrogen Molecule by Hydroxo-/Sulfido-Bridged Rutheniumâ€“Germanium Dinuclear Complex. Theoretical Insights. Inorganic Chemistry, 2015, 54, 576-585.	4.0	9
65	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
66	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
67	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
68	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
69	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.	2.0	28
70	Catalytic Transfer Hydrogenation by a Trivalent Phosphorus Compound: Phosphorusâ€Ligand Cooperation Pathway or P^{III}/P^V Redox Pathway?. Angewandte Chemie - International Edition, 2014, 53, 4633-4637.	13.8	57
71	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
72	Efficient Catalyst for Acceptorless Alcohol Dehydrogenation: Interplay of Theoretical and Experimental Studies. ACS Catalysis, 2014, 4, 1010-1020.	11.2	151

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73	Self-Accelerating CO Sorption in a Soft Nanoporous Crystal. Science, 2014, 343, 167-170.	12.6	434
74	Synthesis, Geometry, and Bonding Nature of Heptacoordinate Compounds of Silicon and Germanium Featuring Three Phosphine Donors. Organometallics, 2014, 33, 6557-6567.	2.3	24
75	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
76	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
77	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
78	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
79	Nickel-Catalyzed Double Carboxylation of Alkynes Employing Carbon Dioxide. Organic Letters, 2014, 16, 4960-4963.	4.6	96
80	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
81	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
82	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
83	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
84	Factors Controlling the Reactivity of Heteroarenes in Direct Arylation with Arylpalladium Acetate Complexes. Organometallics, 2013, 32, 4423-4430.	2.3	47
85	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
86	A theoretical study of luminescent vapochromic compounds including an AuCu2(NHC)2 core. Dalton Transactions, 2013, 42, 4809.	3.3	7
87	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
88	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
89	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
90	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

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91	Levoglucosan Formation from Crystalline Cellulose: Importance of a Hydrogen Bonding Network in the Reaction. ChemSusChem, 2013, 6, 2356-2368.	6.8	74
92	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
93	Complicated Electronic Process of Câ€“C Ïƒ-Bond Activation of Cyclopropene by Ruthenium and Iridium Complexes: Theoretical Study. Organometallics, 2012, 31, 8189-8199.	2.3	5
94	Theoretical Study of Dihydrogen Activation by a Trinuclear Ruthenium Î¼3-Imido Complex. Organometallics, 2012, 31, 5342-5348.	2.3	7
95	Theoretical Study on the Transition-Metal Oxoboryl Complex: Mâ€“BO Bonding Nature, Mechanism of the Formation Reaction, and Prediction of a New Oxoboryl Complex. Inorganic Chemistry, 2012, 51, 4597-4605.	4.0	32
96	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
97	Syntheses and Luminescent Properties of 3,5-Diphenylpyrazolato-Bridged Heteropolynuclear Platinum Complexes. The Influence of Chloride Ligands on the Emission Energy Revealed by the Systematic Replacement of Chloride Ligands by 3,5-Dimethylpyrazolate. Inorganic Chemistry, 2012, 51, 7977-7992.	4.0	29
98	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
99	Theoretical Study of Ïƒ-Bond Activation Reactions and Catalytic Reactions by Transition Metal Complexes. , 2012, , 391-434.		7
100	Theoretical study on aquation reaction of cis-platin complex: RISMâ€“SCFâ€“SEDD, a hybrid approach of accurate quantum chemical method and statistical mechanics. Dalton Transactions, 2011, 40, 11125.	3.3	20
101	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
102	Theoretical Study of Magnesium Fluoride in Aqueous Solution. Journal of Physical Chemistry B, 2011, 115, 10553-10559.	2.6	13
103	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
104	Solvation structure of coroneneâ€“transition metal complex: a RISM-SCF study. Physical Chemistry Chemical Physics, 2011, 13, 309-313.	2.8	20
105	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
106	Synthesis, Structure, and Bonding Nature of Ethynediyl-Bridged Bis(silylene) Dinuclear Complexes of Tungsten and Molybdenum. Organometallics, 2011, 30, 4515-4531.	2.3	22
107	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
108	Theoretical and computational studies of organometallic reactions: successful or not?. Chemical Record, 2010, 10, 29-45.	5.8	31

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109	Experimental and Theoretical Study of a Tungsten Dihydride Silyl Complex: New Insight into Its Bonding Nature and Fluxional Behavior. Organometallics, 2010, 29, 6267-6281.	2.3	23
110	Aqueous Solvation of p-Aminobenzonitrile in the Excited States: A Molecular Level Theory on Density Dependence. Journal of Physical Chemistry B, 2010, 114, 910-914.	2.6	15
111	RISM-SCF-SEDD Study on the Symmetry Breaking of Carbonate and Nitrate Anions in Aqueous Solution. Journal of Physical Chemistry B, 2010, 114, 10513-10519.	2.6	28
112	Theoretical Study of Excited States of Pyrazolate- and Pyridinethiolate-Bridged Dinuclear Platinum(II) Complexes: Relationship between Geometries of Excited States and Phosphorescence Spectra. Inorganic Chemistry, 2010, 49, 8977-8985.	4.0	25
113	Theoretical Study of 1,6-Anhydrosugar Formation from Phenyld-Glucosides under Basic Condition: Reasons for Higher Reactivity of Î²-Anomer. Journal of Organic Chemistry, 2010, 75, 8400-8409.	3.2	9
114	{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
115	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
116	Ab initio study on SN2 reaction of methyl p-nitrobenzenesulfonate and chloride anion in [mmim][PF6]. Physical Chemistry Chemical Physics, 2010, 12, 1822.	2.8	23
117	Analytical energy gradient for reference interaction site model self-consistent field explicitly including spatial electron density distribution. Journal of Chemical Physics, 2009, 131, 214504.	3.0	40
118	Generalization of the New Resonance Theory: Second Quantization Operator, Localization Scheme, and Basis Set. Journal of Chemical Theory and Computation, 2009, 5, 1741-1748.	5.3	10
119	A systematic understanding of orbital energy shift in polar solvent. Journal of Chemical Physics, 2009, 130, 044107.	3.0	12
120	Luminescent Heteropolynuclear Complexes of 3,5â€Dimethylpyrazolate [Pt₂Au₂M₂(Me₂pz)₈] (M=Ag, Cu) Showing the Synergistic Effect of Three Transition Elements in the Excited State. Chemistry - A European Journal, 2009, 15, 4238-4242.	3.3	28
121	Bidirectional Chemoâ€Switching of Spin State in a Microporous Framework. Angewandte Chemie - International Edition, 2009, 48, 4767-4771.	13.8	474
122	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
123	A theoretical study of the liquid structure of nitromethane with RISM method. Journal of Molecular Liquids, 2009, 147, 9-12.	4.9	11
124	Theoretical Study of Dioxygen Binding Process in Iron(III) Catechol Dioxygenase: â€œOxygen Activationâ€• vs â€œSubstrate Activationâ€• Journal of Physical Chemistry B, 2009, 113, 4826-4836.	2.6	17
125	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.	4.0	37
126	First Principle Theory for pK_a Prediction at Molecular Level: pH Effects Based on Explicit Solvent Model. Journal of Physical Chemistry B, 2009, 113, 10509-10514.	2.6	13

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127	How to Stabilize Î·³-Silapropargyl/Alkynylsilyl Complex of [CpL₂M]⁺(L = CO, PMe₃, or PF₃ and M =) Tj ET Q q 1 1 0.284314 rg E		
128	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
129	Thermal Degradation of Methyl Î²-<scp>d</scp>-Glucoside. A Theoretical Study of Plausible Reaction Mechanisms. Journal of Organic Chemistry, 2009, 74, 6891-6894.	3.2	65
130	New Palladium(II) Complex of P,S-Containing Hybrid Calixphyrin. Theoretical Study of Electronic Structure and Reactivity for Oxidative Addition. Journal of the American Chemical Society, 2009, 131, 10955-10963.	13.7	32
131	Carbon dioxide capture at the molecular level. Physical Chemistry Chemical Physics, 2009, 11, 8556.	2.8	33
132	A Theoretical Study of Nickel(0)-Catalyzed Phenylcyanation of Alkynes. Reaction Mechanism and Regioselectivity. Organometallics, 2009, 28, 2583-2594.	2.3	60
133	Theoretical prediction of Oâ€“H, Siâ€“H, and Siâ€“C Ïƒ-bond activation reactions by titanium(IV)â€“imido complex. Canadian Journal of Chemistry, 2009, 87, 1415-1424.	1.1	6
134	A Theoretical Analysis of a Dielsâ^'Alder Reaction in Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 8227-8230.	2.6	47
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