Mitsutaka Okumura

List of Publications by Year in Descending Order

320 papers	9,092 citations	50 h-index	83 g-index
338 ext. papers	9,671 ext. citations	3.6 avg, IF	5.93 L-index

#	Paper	IF	Citations
320	Can we enhance diradical character using interaction with stoichiometric surfaces of ionic oxides? A theoretical investigation using chemical indices. *Physical Chemistry Chemical Physics*, **2021**, 23, 25024-25028	3.6	1
319	Strong Metal–Support Interaction in Pd/Ca2AlMnO5+δ Catalytic NO Reduction over Mn-Doped CaO Shell. *ACS Catalysis*, **2021**, 11, 7996-8003	13.1	2
318	Gibbs Energy of Hydrogen Adsorption on Pt Surface by Machine Learning Potential and Metadynamics. *Chemistry Letters*, **2021**, 50, 1329-1332	1.7	
317	Effect of surface interactions on spin contamination errors of homogeneous spin dimers, chains, and films: model calculations of Au/MgO and Au/BaO systems. *Molecular Physics*, **2021**, 119, e1791989	1.7	4
316	Relative stability among intermediate structures in S2 state of CaMn4O5 cluster in PSII by using hybrid-DFT and DLPNO-CC methods and evaluation of magnetic interactions between Mn ions. *Journal of Photochemistry and Photobiology A: Chemistry*, **2021**, 405, 112923	4.7	3
315	Electron Density-based Estimation of Diradical Character: An Easy Scheme for DFT/Plane-wave Calculations. *Chemistry Letters*, **2021**, 50, 392-396	1.7	2
314	Estimation of spin contamination errors in DFT/plane-wave calculations of solid materials using approximate spin projection scheme. *Chemical Physics Letters*, **2021**, 765, 138291	2.5	7
313	Partial oxidation of propylene with H2 and O2 over Au supported on ZrO2 with different structural and surface properties. *Journal of Catalysis*, **2021**, 401, 188-199	7.3	2
312	Pt/CeO2 with residual chloride as reusable soft Lewis acid catalysts: Application to highly efficient isomerization of allylic esters. *Applied Catalysis B: Environmental*, **2021**, 296, 120333	21.8	3
311	Excellent Catalytic Activity of a Pd-Promoted MnOx Catalyst for Purifying Automotive Exhaust Gases. *ChemCatChem*, **2020**, 12, 4276-4280	5.2	9
310	Clarification of the Relationship between the Magnetic and Conductive Properties of Infinite Chains in Trioxotriangulene Radical Crystals by Spin-Projected DFT/Plane-Wave Calculations. *Advanced Theory and Simulations*, **2020**, 3, 2000050	3.5	6
309	UNO(ULO) active space for multireference calculations on classical and quantum computers. Revisit to the iron-sulfur complexes. *Chemical Physics Letters*, **2020**, 746, 137252	2.5	2
308	Facile NO-CO elimination over zirconia-coated Cu(1□1□0) surfaces: Further evidence from DFT+U calculations. *Applied Surface Science*, **2020**, 508, 145252	6.7	3
307	Electronic and spin structures of CaMnO clusters in the S state of the oxygen evolving complex of photosystem II. Domain-based local pair natural orbital (DLPNO) coupled-cluster (CC) calculations using optimized geometries and natural orbitals (UNO) by hybrid density functional theory (HDFT) calculations. *Physical Chemistry Chemical Physics*, **2020**, 22, 27191-27205	3.6	3
306	Theory of chemical bonds in metalloenzymes XXIV electronic and spin structures of FeMoco and Fe-S clusters by classical and quantum computing. *Molecular Physics*, **2020**, 118, e1760388	1.7	3
305	Comparison of Effective Exchange Integrals of H-H and H-He-H Chains vs. Single Molecules: A Theoretical Study. *Chemistry Letters*, **2020**, 49, 137-140	1.7	5
304	DFT Study for Selective Adsorption of 1,3-Dimethyltrisulfane Responsible for Aged Odor in Japanese Sake Using Supported Gold Nanoparticles. *Chemistry Letters*, **2020**, 49, 218-221	1.7	

303	Theoretical Investigation of the Heterojunction Effect on the Catalytic Activity and Selectivity of an Core-Shell Catalyst in Aerobic Oxidation. *Journal of Physical Chemistry C*, **2020**, 124, 17039-17047	3.8	5
302	Theoretical study of selective hydrogenolysis of methyl vinyl carbinol over Au-Ni bimetallic catalyst: Toward constructing a working hypothesis for the role of dichloroethane solvent and perimeter sites. *Chemical Physics Letters*, **2020**, 754, 137773	2.5	
301	Domain-based local pair natural orbital CCSD(T) calculations of strongly correlated electron systems: Examination of dynamic equilibrium models based on multiple intermediates in S1 state of photosystem II. *Molecular Physics*, **2020**, 118, e1666171	1.7	3
300	Spin contamination errors on spin-polarized density functional theory/plane-wave calculations for crystals of one-dimensional materials. *Applied Physics Express*, **2019**, 12, 115506	2.4	19
299	Domain-based local pair natural orbital CCSD(T) calculations of six different S1 structures of oxygen evolving complex of photosystem II. Proposal of multi-intermediate models for the S1 state. *Chemical Physics Letters*, **2019**, 732, 136660	2.5	9
298	Effect of spin contamination error on surface catalytic reaction: NO reduction by core-shell catalysts. *Molecular Physics*, **2019**, 117, 2251-2259	1.7	18
297	Theoretical study of aerobic oxidation of alcohols over Au38 nanocluster by a two-step-modeling approach. *Chemical Physics Letters*, **2019**, 724, 115-121	2.5	6
296	Theoretical and computational investigations of geometrical, electronic and spin structures of the CaMn O (X = 5, 6) cluster in the Kok cycle S (i = 0-3) of oxygen evolving complex of photosystem II. *Physiologia Plantarum*, **2019**, 166, 44-59	4.6	8
295	Extent of Spin Contamination Errors in DFT/Plane-wave Calculation of Surfaces: A Case of Au Atom Aggregation on a MgO Surface. *Molecules*, **2019**, 24,	4.8	19
294	Effect of ceria and zirconia supports on NO reduction over platinum-group metal catalysts: A DFT study with comparative experiments. *Catalysis Today*, **2019**, 332, 236-244	5.3	13
293	Domain-based local pair natural orbital CCSD(T) calculations of fourteen different S2 intermediates for water oxidation in the Kok cycle of OEC of PSII. Re-visit to one LS-two HS model for the S2 state. *Chemical Physics Letters*, **2019**, 734, 136731	2.5	10
292	NO-CO Reaction Over Metal-supported Ultrathin Oxide Films: Evaluating Novel Catalysts by Density-functional Theory Calculations. *Journal of Computer Chemistry Japan*, **2019**, 18, 1-8	0.2	
291	Theoretical study on the electronic structure of [4Fe-4S] cluster **2019**, 499-502		
290	Dynamic Gate Opening of ZIF-8 for Bulky Molecule Adsorption as Studied by Vapor Adsorption Measurements and Computational Approach. *Journal of Physical Chemistry C*, **2019**, 123, 27542-27553	3.8	13
289	Theoretical study of correlations between the coordination structures and catalytic activities in polymer-stabilized au nanocluster catalysts. *Journal of Computational Chemistry*, **2019**, 40, 222-228	3.5	9
288	UNO DMRG CAS CI calculations of binuclear manganese complex Mn(IV) O (NHCHCO) : Scope and applicability of Heisenberg model. *Journal of Computational Chemistry*, **2019**, 40, 333-341	3.5	13
287	Free energy reaction root mapping of alanine tripeptide in water. *Molecular Physics*, **2019**, 117, 2284-2292	1.7	3
286	Theoretical investigation of the effect of phosphate doping on the aggregation of Au atoms on an Al2O3 (0001) surface. *Applied Surface Science*, **2019**, 465, 1003-1013	6.7	4

285	Dielectric Jump and Negative Electrostriction in Metallosupramolecular Ionic Crystals. *Scientific Reports*, **2018**, 8, 2606	4.9	8
284	Carbon Monoxide Oxidation by Polyoxometalate-Supported Gold Nanoparticulate Catalysts: Activity, Stability, and Temperature- Dependent Activation Properties. *Angewandte Chemie*, **2018**, 130, 1539-1543	3.6	15
283	Carbon Monoxide Oxidation by Polyoxometalate-Supported Gold Nanoparticulate Catalysts: Activity, Stability, and Temperature- Dependent Activation Properties. *Angewandte Chemie - International Edition*, **2018**, 57, 1523-1527	16.4	17
282	Clarification of the interaction between Au atoms and the anatase TiO2 (112) surface using density functional theory. *Surface Science*, **2018**, 670, 23-32	1.8	9
281	Estimation of spin contamination error in dissociative adsorption of Au2 onto MgO(0 0 1) surface: First application of approximate spin projection (AP) method to plane wave basis. *Chemical Physics Letters*, **2018**, 701, 103-108	2.5	19
280	Adsorption and thermal reactivity of dimethyl trisulfide on a Au(111) single-crystal surface. *Surface Science*, **2018**, 677, 186-192	1.8	2
279	Toward a translational molecular ratchet: face-selective translation coincident with deuteration in a pseudo-rotaxane. *Scientific Reports*, **2018**, 8, 8950	4.9	12
278	TiO2 Crystal Structure Dependence of Low-temperature CO Oxidation Catalyzed by Au/TiO2. *Chemistry Letters*, **2018**, 47, 200-203	1.7	6
277	Au Atom Diffusions on Reduced and Cl-Adsorbed Rutile TiO2(110) Surfaces: A DFT + U Study. *E-Journal of Surface Science and Nanotechnology*, **2018**, 16, 267-273	0.7	0
276	Automated Search of Minimum Free-Energy Path by Umbrella Integration. *Journal of Computational Chemistry*, **2018**, 39, 1913-1921	3.5	3
275	Automated Exploration of Free Energy Landscapes Based on Umbrella Integration. *International Journal of Molecular Sciences*, **2018**, 19,	6.3	7
274	Theoretical Investigation of Surface Oxidation of NiO/Au Core-Shell Catalyst. *E-Journal of Surface Science and Nanotechnology*, **2018**, 16, 242-246	0.7	4
273	Selective adsorption of 1,3-dimethyltrisulfane (DMTS) responsible for aged odour in Japanese sake using supported gold nanoparticles. *Scientific Reports*, **2018**, 8, 16064	4.9	2
272	Relative stability between the manganese hydroxide- and oxo-models for water oxidation by CCSD, DMRG CASCI, CASSCF, CASPT2 and CASDFT methods; Importance of static and dynamical electron correlation effects for OEC of PSII. *Chemical Physics Letters*, **2018**, 705, 85-91	2.5	8
271	Potential of Titania-covered Ag Catalysts for NOx Reduction: A DFT Study. *Chemistry Letters*, **2017**, 46, 456-459	1.7	14
270	Theoretical Clarification of the Coexistence of Cl Effects on Au/TiO2: The Interaction between Au Clusters and the TiO2 Surface, and the Aggregation of Au Clusters on the TiO2 Surface. *Bulletin of the Chemical Society of Japan*, **2017**, 90, 506-519	5.1	14
269	Assessment of semi-empirical molecular orbital calculations for describing magnetic interactions. *Polyhedron*, **2017**, 136, 52-57	2.7	6
268	Ab initio computations of zero-field splitting parameters and effective exchange integrals for single-molecule magnets (Mn 12 - and Mn 11 Cr-acetate clusters). *Polyhedron*, **2017**, 136, 159-169	2.7	1

267	Density functional study of the magneto-structural correlations of manganese complexes, [Mn2O2H (salpn)2]+(2)(n= 0,2) from the viewpoint of the protonation modes of the bridging oxygen anions. *Polyhedron*, **2017**, 136, 102-109	2.7	1
266	High NOx Reduction Activity of an Ultrathin Zirconia Film Covering a Cu Surface: A DFT Study. *Catalysis Letters*, **2017**, 147, 1827-1833	2.8	16
265	Quantum mechanics study on synthetic model of copper-containing quercetin 2,4-dioxygenase. *Polyhedron*, **2017**, 136, 45-51	2.7	0
264	UNO DMRG CASCI calculations of effective exchange integrals for m-phenylene-bis-methylene spin clusters. *Molecular Physics*, **2017**, 115, 2154-2167	1.7	2
263	Effects of halogens on interactions between a reduced TiO 2 (110) surface and noble metal atoms: A DFT study. *Applied Surface Science*, **2017**, 411, 149-162	6.7	14
262	Theoretical study on relationship between spin structure and electron conductivity of one-dimensional tri-nickel(II) complex. *Polyhedron*, **2017**, 136, 125-131	2.7	6
261	Chloride-free and water-soluble Au complex for preparation of supported small nanoparticles by impregnation method. *Journal of Catalysis*, **2017**, 353, 74-80	7.3	9
260	Full-valence density matrix renormalisation group calculations on meta-benzyne based on unrestricted natural orbitals. Revisit of seamless continuation from broken-symmetry to symmetry-adapted models for diradicals. *Molecular Physics*, **2017**, 115, 2267-2284	1.7	11
259	Valence Interconversion of Octahedral Nickel(II/III/IV) Centers. *Angewandte Chemie - International Edition*, **2017**, 56, 13762-13766	16.4	13
258	Valence Interconversion of Octahedral Nickel(II/III/IV) Centers. *Angewandte Chemie*, **2017**, 129, 13950-13954	3.6	4
257	Theoretical Investigation for Heterojunction Effects in Polymer-stabilized Au Nanocluster Catalysis: Difference in Catalytic Activity between Au:PVP and Au:PAA. *Chemistry Letters*, **2016**, 45, 344-346	1.7	10
256	Theoretical Studies on the Magnetic and Conductive Properties of Crystals Containing Open-Shell Trioxotriangulene Radicals. *Bulletin of the Chemical Society of Japan*, **2016**, 89, 315-333	5.1	13
255	Advances in Gold Catalysis and Understanding the Catalytic Mechanism. *Chemical Record*, **2016**, 16, 2278-2293	6.6	41
254	Advances in polymer-stabilized Au nano-cluster catalysis : Interplay of theoretical calculations and experiments. *Chinese Journal of Catalysis*, **2016**, 37, 1588-1593	11.3	3
253	Interplay of theoretical calculations and experiments for a study of catalysis by gold. *Catalysis Today*, **2016**, 259, 81-86	5.3	20
252	DFT study of catalytic activity of an ultrathin TiO2(110) layer covering Au(112): O2 activation, CO oxidation, and replacing Au with Ag. *Catalysis Communications*, **2016**, 77, 79-82	3.2	13
251	Linear Response Function of Bond-Order. *International Journal of Molecular Sciences*, **2016**, 17,	6.3	1
250	Crystalline-Amorphous-Crystalline Transformation in a Highly Brilliant Luminescent System with Trigonal-Planar Gold(I) Centers. *Scientific Reports*, **2016**, 6, 26002	4.9	15

249	Computational Study of Catalytic Reaction of Quercetin 2,4-Dioxygenase. *Journal of Physical Chemistry B*, **2015**, 119, 6952-62	3.4	13
248	DFT and TD-DFT studies of electronic structures and one-electron excitation states of a cyanide-bridged molecular square complex. *Inorganic Chemistry Frontiers*, **2015**, 2, 771-779	6.8	14
247	A Career in Catalysis: Masatake Haruta. *ACS Catalysis*, **2015**, 5, 4699-4707	13.1	60
246	Theoretical investigation for isomerization of allylic alcohols over Au6 cluster. *Gold Bulletin*, **2015**, 48, 31-37	1.6	3
245	Density Functional Theory Study of Active Oxygen at the Perimeter of Au/TiO2 Catalysts. *Journal of Physical Chemistry C*, **2015**, 119, 25907-25916	3.8	34
244	Nearsightedness-related indices of finite systems based on linear response function: one-dimensional cases. *Molecular Physics*, **2015**, 1-9	1.7	1
243	Synthesis and catalytic activity of crown jewel-structured (IrPd)/Au trimetallic nanoclusters. *Advanced Materials*, **2015**, 27, 1383-8	24	35
242	Linear response function of the Mayer bond order: an indicator to describe intrinsic chemical reactivity of molecules. *Molecular Physics*, **2015**, 113, 336-341	1.7	3
241	Theory of chemical bonds in metalloenzymes XX: magneto-structural correlations in the CaMn4O5 cluster in oxygen-evolving complex of photosystem II. *Molecular Physics*, **2015**, 1-28	1.7	4
240	Theoretical Study of Electronic Properties of Phenalenyl Radical and Zethrene Diradical Species: Possibility of Triplet Oxygen Adsorption onto Graphene Surface. *Bulletin of the Chemical Society of Japan*, **2015**, 88, 149-161	5.1	8
239	Theoretical Investigation on the Au-Anchor Site in Phosphate-Doped Au/Al2O3 Catalysts. *E-Journal of Surface Science and Nanotechnology*, **2015**, 13, 380-384	0.7	5
238	DFT Study of CO Oxidation Catalyzed by Au/TiO2: Activity of Small Clusters. *E-Journal of Surface Science and Nanotechnology*, **2015**, 13, 129-134	0.7	11
237	QM/MM study of hydrolysis of arginine catalysed by arginase. *Molecular Physics*, **2015**, 1-9	1.7	2
236	Accurate standard hydrogen electrode potential and applications to the redox potentials of vitamin C and NAD/NADH. *Journal of Physical Chemistry A*, **2015**, 119, 369-76	2.8	76
235	Asymmetric dinuclear bis(dipyrrinato)zinc(II) complexes: broad absorption and unidirectional quantitative exciton transmission. *Chemical Communications*, **2014**, 50, 5881-3	5.8	27
234	DFT study of CO oxidation over Au/TiO2(1 1 0): The extent of the reactive perimeter zone. *Chemical Physics Letters*, **2014**, 610-611, 76-81	2.5	20
233	Colloidal Au single-atom catalysts embedded on Pd nanoclusters. *Journal of Materials Chemistry A*, **2014**, 2, 13498-13508	13	51
232	Theory of chemical bonds in metalloenzymes XIX: labile manganese oxygen bonds of the CaMn4O5 cluster in oxygen evolving complex of photosystem II. *Molecular Physics*, **2014**, 112, 485-507	1.7	16

231	DFT and DFT-D studies on molecular structure of double-decker phthalocyaninato-terbium(III) complex. *Molecular Physics*, **2014**, 112, 995-1001	1.7	13
230	Preparation of Agcore/Aushell bimetallic nanoparticles from physical mixtures of Au clusters and Ag ions under dark conditions and their catalytic activity for aerobic glucose oxidation. *Journal of Alloys and Compounds*, **2014**, 586, 462-468	5.7	18
229	Bistable multifunctionality and switchable strong ferromagnetic-to-antiferromagnetic coupling in a one-dimensional rhodium(I)-semiquinonato complex. *Journal of the American Chemical Society*, **2014**, 136, 7026-37	16.4	30
228	Theoretical Investigation on the Optical Properties of Diphosphine-protected Au8 Cluster Complexes. *Chemistry Letters*, **2014**, 43, 880-882	1.7	1
227	Formation of Gold Clusters on La-Ni Mixed Oxides and Its Catalytic Performance for Isomerization of Allylic Alcohols to Saturated Aldehydes. *Chemistry Letters*, **2014**, 43, 1368-1370	1.7	7
226	The translation elongation factor eEF2 is a novel tumor-associated antigen overexpressed in various types of cancers. *International Journal of Oncology*, **2014**, 44, 1461-9	4.4	43
225	Theoretical investigation on nearsightedness of finite model and molecular systems based on linear response function analysis. *Molecules*, **2014**, 19, 13358-73	4.8	3
224	DFT calculations for Au adsorption onto a reduced TiO2 (110) surface with the coexistence of Cl. *Molecular Physics*, **2014**, 112, 365-378	1.7	14
223	DFT calculations for aerobic oxidation of alcohols over neutral Au6 cluster. *Molecular Physics*, **2014**, 112, 385-392	1.7	13
222	Facile Preparation of 1,5-Diazacyclooctanes from Unsaturated Imines: Effects of the Hydroxyl Groups on [4+4] Dimerization. *Synlett*, **2014**, 25, 1026-1030	2.2	15
221	Combination of approximate spin-projection and spin-restricted calculations based on ONIOM method for geometry optimization of large biradical systems. *International Journal of Quantum Chemistry*, **2013**, 113, 290-295	2.1	5
220	Theoretical investigation for the stability of the concave-bound cyclopentadienyl iron complex of sumanene. *International Journal of Quantum Chemistry*, **2013**, 113, 437-442	2.1	7
219	Linear response function approach for the boundary problem of QM/MM methods. *International Journal of Quantum Chemistry*, **2013**, 113, 336-341	2.1	4
218	Full geometry optimizations of the mixed-valence CaMn4O4X(H2O)4 (X=OH or O) cluster in OEC of PS II: Degree of symmetry breaking of the labile Mn-X-Mn bond revealed by several hybrid DFT calculations. *International Journal of Quantum Chemistry*, **2013**, 113, 525-541	2.1	58
217	The nature of chemical bonds of the CaMn4O5 cluster in oxygen evolving complex of photosystem II: Jahn-Teller distortion and its suppression by Ca doping in cubane structures. *International Journal of Quantum Chemistry*, **2013**, 113, 453-473	2.1	59
216	Novel formation of Ag/Au bimetallic nanoparticles by physical mixture of monometallic nanoparticles in dispersions and their application to catalysts for aerobic glucose oxidation. *Langmuir*, **2013**, 29, 10330-9	4	57
215	X-ray magnetic circular dichroism investigation of the electron transfer phenomena responsible for magnetic switching in a cyanide-bridged [CoFe] chain. *Inorganic Chemistry*, **2013**, 52, 13956-62	5.1	17
214	Theoretical studies of electronic structures, magnetic properties and electron conductivities of one-dimensional Ni(n) (n = 3, 5, 7) complexes. *Dalton Transactions*, **2013**, 42, 16200-8	4.3	15

213	meso-Alkynyl BODIPYs: structure, photoproperties, extension, and manipulation of frontier orbitals. *Chemistry - an Asian Journal*, **2013**, 8, 723-7	4.5	21
212	Theory of chemical bonds in metalloenzymes XVIII. Importance of mixed-valence configurations for Mn5O5, CaMn4O5 and Ca2Mn3O5 clusters revealed by UB3LYP computations. A bio-inspired strategy for artificial photosynthesis. *Polyhedron*, **2013**, 57, 138-149	2.7	8
211	Photophysical properties of mono- and di-nuclear platinum(II) complexes with the tridentate ligand 2-phenyl-6-(1H-pyrazol-3-yl)-pyridine: A DFT and TDDFT study. *Journal of Organometallic Chemistry*, **2013**, 743, 163-169	2.3	13
210	DFT calculations for chlorine elimination from chlorine-adsorbed gold clusters by hydrogen. *Chemical Physics Letters*, **2013**, 579, 94-99	2.5	9
209	Reprint of Theory of chemical bonds in metalloenzymes XVIII. Importance of mixed-valence configurations for Mn5O5, CaMn4O5 and Ca2Mn3O5 clusters revealed by UB3LYP computations. A bio-inspired strategy for artificial photosynthesis *Polyhedron*, **2013**, 66, 283-293	2.7	
208	Theory of chemical bonds in metalloenzymes XVI. Oxygen activation by high-valent transition metal ions in native and artificial systems. *Polyhedron*, **2013**, 66, 228-244	2.7	7
207	DFT calculations of effective exchange integrals at the complete basis set limit on oxo-vanadium ring complex. *Polyhedron*, **2013**, 66, 97-101	2.7	6
206	A quantum chemical study on polymerization catalysts for polyesters: Catalytic performance of chelated complexes of titanium. *Polymer*, **2013**, 54, 3297-3305	3.9	8
205	Conjugated trinuclear group-9 metalladithiolenes with a triphenylene backbone. *Inorganic Chemistry*, **2013**, 52, 7411-6	5.1	22
204	A Density Functional Theory Based Protocol to Compute the Redox Potential of Transition Metal Complex with the Correction of Pseudo-Counterion: General Theory and Applications. *Journal of Chemical Theory and Computation*, **2013**, 9, 2974-80	6.4	29
203	Crown Jewel catalyst: How neighboring atoms affect the catalytic activity of top Au atoms?. *Journal of Catalysis*, **2013**, 305, 7-18	7.3	40
202	Diffuse Unoccupied Molecular Orbital of Rubrene Causing Image-Potential State Mediated Excitation. *Journal of Physical Chemistry C*, **2013**, 117, 20098-20103	3.8	19
201	Consistent scheme for computing standard hydrogen electrode and redox potentials. *Journal of Computational Chemistry*, **2013**, 34, 21-6	3.5	30
200	Extraordinary Aggregation of Inorganic Anions in Chiral Metallosupramolecular Ionic Crystals. *Bulletin of the Chemical Society of Japan*, **2013**, 86, 908-920	5.1	39
199	Ab initio DFT study of magneto-structural correlation of dinuclear mixed-valence Mn complexes. *Journal of Physics: Conference Series*, **2013**, 428, 012035	0.3	1
198	How to determine boundaries for QM/MM calculations: A guideline based on linear response function for glutathione. *Journal of Physics: Conference Series*, **2013**, 454, 012055	0.3	1
197	Does B3LYP correctly describe magnetism of manganese complexes with various oxidation numbers and various structural motifs?. *Chemical Physics Letters*, **2012**, 519-520, 134-140	2.5	8
196	A quantum chemical study on the thermal degradation reaction of polyesters. *Polymer Degradation and Stability*, **2012**, 97, 941-947	4.7	7

195	Heterogeneous Catalysis by Gold. *Advances in Catalysis*, **2012**, 55, 1-126	2.4	113
194	Role of perferryl-oxo oxidant in alkane hydroxylation catalyzed by cytochrome P450: a hybrid density functional study. *Journal of Physical Chemistry B*, **2012**, 116, 4713-30	3.4	16
193	Performance of the coupled cluster and DFT methods for through-space magnetic interactions of nitroxide dimer. *Chemical Physics Letters*, **2012**, 542, 19-25	2.5	10
192	Electronic and Spin Structures of the CaMn4O5(H2O)4 Cluster in OEC of PSII Refined to 1.9 Å X-ray Resolution. *Advances in Quantum Chemistry*, **2012**, 64, 121-187	1.4	30
191	Efficient synthesis of 2,6,9-triazabicyclo[3.3.1]nonanes through amine-mediated formal [4+4] reaction of unsaturated imines. *Tetrahedron Letters*, **2012**, 53, 5899-5902	2	18
190	Fluorescent azadipyrrinato zinc(II) complex: hybridisation with a dipyrrinato ligand. *Dalton Transactions*, **2012**, 41, 14035-7	4.3	25
189	Possible mechanisms of water splitting reaction based on proton and electron release pathways revealed for CaMn4O5 cluster of PSII refined to 1.9 Å X-ray resolution. *International Journal of Quantum Chemistry*, **2012**, 112, 253-276	2.1	63
188	Theory of chemical bonds in metalloenzymes. XVII. Symmetry breaking in manganese cluster structures and chameleonic mechanisms for the O?O bond formation of water splitting reaction. *International Journal of Quantum Chemistry*, **2012**, 112, 121-135	2.1	19
187	Structure and reactivity of the mixed-valence CaMn4O5(H2O)4 and CaMn4O4(OH)(H2O)4 clusters at oxygen evolution complex of photosystem II. Hybrid DFT (UB3LYP and UBHandHLYP) calculations. *International Journal of Quantum Chemistry*, **2012**, 112, 321-343	2.1	46
186	An extremely bright heteroleptic bis(dipyrrinato)zinc(II) complex. *Chemistry - an Asian Journal*, **2012** , 7, 907-10	4.5	61
185	Locality and nonlocality of electronic structures of molecular systems: Toward QM/MM and QM/QM approaches **2012**,		2
184	Theory of chemical bonds in metalloenzymes - Manganese oxides clusters in the oxygen evolution center - **2012**,		7
183	Catalytically highly active top gold atom on palladium nanocluster. *Nature Materials*, **2011**, 11, 49-52	27	486
182	Modification of MOF catalysts by manipulation of counter-ions: experimental and theoretical studies of photochemical hydrogen production from water over microporous diruthenium (II, III) coordination polymers. *Supramolecular Chemistry*, **2011**, 23, 287-296	1.8	29
181	Electron Conductivity in Modified Models of Artificial Metal–DNA Using Green's Function-Based Elastic Scattering Theory. *Bulletin of the Chemical Society of Japan*, **2011**, 84, 366-375	5.1	7
180	MicroRNA-mediated downregulation of mTOR/FGFR3 controls tumor growth induced by Src-related oncogenic pathways. *Oncogene*, **2011**, 30, 3489-501	9.2	87
179	Theoretical study of intra- and inter-chain magnetic interactions in [Ni(chxn)2Br]Br2. *Polyhedron*, **2011**, 30, 3116-3120	2.7	6
178	Continuous optimization methods for ground-state searches of spin clusters. *Polyhedron*, **2011**, 30, 3218-3223	2.7	23

177	Theoretical study on singlet oxygen adsorption onto surface of graphene-like aromatic hydrocarbon molecules. *Polyhedron*, **2011**, 30, 3249-3255	2.7	8
176	Ab initio study of magnetic interactions of manganese-oxide clusters. *Polyhedron*, **2011**, 30, 3256-3261	2.7	16
175	Theoretical studies of d□ and d□ magnetic interactions in (EDT-TTFVO)2FeBr4 crystals. *Polyhedron*, **2011**, 30, 3284-3291	2.7	3
174	Theoretical studies of host□guest interaction in the cavity of the nanoporous [Rh2bza4pyz]n crystal. *Polyhedron*, **2011**, 30, 3292-3297	2.7	
173	Singlet□triplet energy gap for trimethylenemethane, oxyallyl diradical, and related species: single- and multireference computational results. *Theoretical Chemistry Accounts*, **2011**, 130, 739-748	1.9	30
172	Symmetry and broken symmetry in molecular orbital description of unstable molecules IV: comparison between single- and multi-reference computational results for antiaromtic molecules. *Theoretical Chemistry Accounts*, **2011**, 130, 749-763	1.9	36
171	Labile electronic and spin states of the CaMn4O5 cluster in the PSII system refined to the 1.9 □ X-ray resolution. UB3LYP computational results. *Chemical Physics Letters*, **2011**, 506, 98-103	2.5	63
170	Potential energy curve for ring-opening reactions: comparison between broken-symmetry and multireference coupled cluster methods. *Journal of Physical Chemistry A*, **2011**, 115, 5625-31	2.8	12
169	Theoretical studies on the structural and magnetic property of arginase active site. *Supramolecular Chemistry*, **2011**, 23, 22-28	1.8	3
168	Theoretical study of absorption spectrum of dirhodium tetracarboxylate complex [Rh2(CH3COO)4(H2O)2] in aqueous solution revisited. *Supramolecular Chemistry*, **2011**, 23, 329-336	1.8	6
167	Stable Dispersions of PVP-Protected Au/Pt/Ag Trimetallic Nanoparticles as Highly Active Colloidal Catalysts for Aerobic Glucose Oxidation. *Journal of Physical Chemistry C*, **2011**, 115, 14883-14891	3.8	77
166	Unique structural and electronic features of perferryl-oxo oxidant in Cytochrome P450. *Journal of Physical Chemistry B*, **2011**, 115, 10730-8	3.4	23
165	Broken-symmetry natural orbital (BSNO)□Mk-MRCC study on the exchange coupling in the binuclear copper(II) compounds. *Chemical Physics Letters*, **2011**, 505, 11-15	2.5	20
164	Possible mechanisms for the O□O bond formation in oxygen evolution reaction at the CaMn4O5(H2O)4 cluster of PSII refined to 1.9□X-ray resolution. *Chemical Physics Letters*, **2011**, 511, 138-145	2.5	91
163	A quantum chemical study on the polycondensation reaction of polyesters: The mechanism of catalysis in the polycondensation reaction. *Polymer*, **2011**, 52, 3443-3450	3.9	17
162	Theoretical studies on the electronic structure of the synthetic complex of soluble methanemonooxygenase intermediate Q. *Supramolecular Chemistry*, **2011**, 23, 83-87	1.8	2
161	MkMRCC, APUCC, APUBD calculations of didehydronated species: comparison among calculated through-bond effective exchange integrals for diradicals. *Molecular Physics*, **2010**, 108, 2533-2541	1.7	10
160	Reinvestigation of the reaction of ethylene and singlet oxygen by the approximate spin projection method. Comparison with multireference coupled-cluster calculations. *Journal of Physical Chemistry A*, **2010**, 114, 7967-74	2.8	37

159	Multireference character of 1,3-dipolar cycloaddition of ozone with ethylene and acrylonitrile. *Journal of Physical Chemistry A*, **2010**, 114, 12116-23	2.8	22
158	MkMRCC, APUCC and APUBD approaches to 1,n-didehydropolyene diradicals: the nature of through-bond exchange interactions. *Molecular Physics*, **2010**, 108, 2559-2578	1.7	11
157	Hydrogen Production from Water Using Novel Three-dimensional Interpenetrated ZnPd Coordination Polymer. *Chemistry Letters*, **2010**, 39, 878-880	1.7	15
156	Photocatalytic Hydrogen Production from Water Using Heterogeneous Two-dimensional Rhodium Coordination Polymer [Rh2(p-BDC)2]n. *Chemistry Letters*, **2010**, 39, 358-359	1.7	42
155	Theoretical Study on the Electronic Configurations and Nature of Chemical Bonds of Dirhodium Tetraacetato Complexes [Rh2(CH3COO)4(L)2] (L = H2O, Free): Broken Symmetry Approach. *Bulletin of the Chemical Society of Japan*, **2010**, 83, 1481-1488	5.1	8
154	A broken-symmetry study on the automerization of cyclobutadiene. Comparison with UNO- and DNO-MRCC methods. *Chemical Physics Letters*, **2010**, 498, 253-258	2.5	18
153	Which hybrid GGA DFT is suitable for Cu2O2 systems if the spin contamination error is removed?. *Chemical Physics*, **2010**, 368, 1-6	2.3	23
152	Theoretical studies of the effect of orientation of ligands and spin contamination error on the chemical bonding in the FeO2 core in oxymyoglobin. *Computational and Theoretical Chemistry*, **2010**, 954, 98-104		3
151	Sequence-dependent proton-transfer reaction in stacked GC pair III: The influence of proton transfer to conductivity. *International Journal of Quantum Chemistry*, **2010**, 110, 2221-2230	2.1	5
150	DFT calculations for the heterojunction effect between metal clusters and the stabilizer molecules. *International Journal of Quantum Chemistry*, **2010**, 110, 2903-2911	2.1	5
149	Development of approximately spin projected energy derivatives for biradical systems. *International Journal of Quantum Chemistry*, **2010**, 110, 3053-3060	2.1	4
148	UNO- and ULO-MRCC(Mk), AP-UCC and AP-UBD approaches to diradical systems. *International Journal of Quantum Chemistry*, **2010**, 110, 3015-3026	2.1	15
147	Theory of chemical bonds in metalloenzymes. XV. Local singlet and triplet diradical mechanisms for radical coupling reactions in the oxygen evolution complex. *International Journal of Quantum Chemistry*, **2010**, 110, 3101-3128	2.1	46
146	Theory of chemical bonds in metalloenzymes. XIV. Correspondence between magnetic coupling mode and radical coupling mechanism in hydroxylations with methane monooxygenase and related species. *International Journal of Quantum Chemistry*, **2010**, 110, 2955-2981	2.1	14
145	Instability In Chemical Bonds: Uno Cascc, Resonating Ucc And Approximately Projected Ucc Methods To Quasi-Degenerate Electronic Systems. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 621-648	0.7	1
144	A kinetic study on the low temperature oxidation of CO over Ag-contaminated Au fine powder. *Journal of Catalysis*, **2009**, 262, 280-286	7.3	34
143	Hydrogen Dissociation by Gold Clusters. *Angewandte Chemie*, **2009**, 121, 9679-9682	3.6	53
142	Hydrogen dissociation by gold clusters. *Angewandte Chemie - International Edition*, **2009**, 48, 9515-8	16.4	253

141	BS DFT and BS HDFT studies of Cr?Cr sextuple bond from the viewpoint of electron correlation effects. *International Journal of Quantum Chemistry*, **2009**, 109, 3315-3324	2.1	9
140	Theory of chemical bonds in metalloenzymes XIII: Singlet and triplet diradical mechanisms of hydroxylations with iron-oxo species and P450 are revisited. *International Journal of Quantum Chemistry*, **2009**, 109, 3723-3744	2.1	9
139	Estimation of effective exchange integral value of polyradical systems based on the band calculation. *International Journal of Quantum Chemistry*, **2009**, 109, 3632-3640	2.1	5
138	Extended Hartree□Fock theory of chemical reactions. IX. Diradical and perepoxide mechanisms for oxygenations of ethylene with molecular oxygen and iron-oxo species are revisited. *International Journal of Quantum Chemistry*, **2009**, 109, 3745-3766	2.1	12
137	Approximately spin-projected Hessian for broken symmetry method and stretching frequencies of F2 and singlet O2. *International Journal of Quantum Chemistry*, **2009**, 109, 3641-3648	2.1	11
136	Theoretical studies on chemical bonding between Cu(II) and oxygen molecule in type 3 copper proteins. *International Journal of Quantum Chemistry*, **2009**, 109, 3649-3658	2.1	9
135	Resonating coupled-cluster CI approach to ion-radical systems: Comparison with the unrestricted coupled-cluster approach. *International Journal of Quantum Chemistry*, **2009**, 109, 3811-3818	2.1	7
134	A resonating broken-symmetry CI study of cationic states of phenalenyl dimeric compounds. *Polyhedron*, **2009**, 28, 1628-1633	2.7	4
133	Theoretical calculations of the pressure effect for the □phase of p-NPNN. *Polyhedron*, **2009**, 28, 1898-1902	2.7	3
132	Theoretical studies on electronic structures and magnetic interactions of K4[Pt2(pop)4X] □2H2O (X = Cl, Br) complexes. *Polyhedron*, **2009**, 28, 1668-1671	2.7	4
131	Theoretical studies on magnetic interactions between Cu(II) ions in hydroxypyridone nucleobases. *Polyhedron*, **2009**, 28, 1714-1717	2.7	9
130	Theoretical studies on magnetic interactions between Cu(II) ions in salen nucleobases. *Polyhedron*, **2009**, 28, 1945-1949	2.7	12
129	Theoretical study of magnetic interaction between C60 anion radicals. *Polyhedron*, **2009**, 28, 1750-1753	2.7	3
128	Theoretical calculations of magnetic properties of the □ □ □and □phases of p-NPNN. *Polyhedron* , **2009**, 28, 1768-1775	2.7	2
127	Theory of chemical bonds in metalloenzymes XII: Electronic and spin structures of metallo□xo and isoelectronic species and spin crossover phenomena in oxygenation reactions. *Polyhedron*, **2009**, 28, 2044-2052	2.7	8
126	Quantum dynamic simulations for single molecular magnets using anisotropic spin models. *Polyhedron*, **2009**, 28, 2092-2096	2.7	5
125	Theoretical investigation of the interaction between oxygen molecules and small Au clusters using approximately spin-projected geometry optimization (AP-opt) method. *Catalysis Today*, **2009**, 143, 282-285	5.3	18
124	Transition state optimization based on approximate spin-projection (AP) method. *Chemical Physics Letters*, **2009**, 483, 168-171	2.5	58

123	Theoretical studies on sulfur and metal cation (Cu(II), Ni(II), Pd(II), and Pt(II))-containing artificial DNA. *Journal of Physical Chemistry B*, **2009**, 113, 12790-5	3.4	8
122	Syntheses, structures and solid-state properties of MMX mixed-valence chains, [Ni(II/III)2(RCS2)4I]infinity (R = Et, n-Pr and n-Bu): evidence of a spin-Peierls transition. *Inorganic Chemistry*, **2009**, 48, 6680-91	5.1	43
121	Symmetry and broken-symmetry in molecular orbital descriptions of unstable molecules. 3. The nature of chemical bonds of spin frustrated systems. *Journal of Physical Chemistry A*, **2009**, 113, 15281-97	2.8	9
120	Theoretical investigation of thermal decomposition of peroxidized coelenterazines with and without external perturbations. *Journal of Physical Chemistry A*, **2009**, 113, 15171-87	2.8	9
119	Spin contamination error in optimized geometry of singlet carbene ((1)A1) by broken-symmetry method. *Journal of Physical Chemistry A*, **2009**, 113, 15041-6	2.8	57
118	Instability in Chemical Bonds from Broken-Symmetry Single-Reference to Symmetry-Adapted Multireference Approaches to Strongly Correlated Electron Systems **2009**,		7
117	Theoretical investigation of the magnetic interactions of Ni9 complexes. *Journal of Physical Chemistry A*, **2008**, 112, 4020-8	2.8	7
116	3P-111 Theoretical studies on the electronic structure of the active site of Tyrosinase(The 46th Annual Meeting of the Biophysical Society of Japan). *Seibutsu Butsuri*, **2008**, 48, S144	0	
115	DFT studies of the characteristics of Pd□Pt core-shell clusters. *Research on Chemical Intermediates*, **2008**, 34, 737-742	2.8	4
114	N-bands Hubbard models. IV. Comparisons of electron- or hole-doped quaternary oxypictides LaOMPn superconductors with cuprates. *International Journal of Quantum Chemistry*, **2008**, 108, 3016-3041	2.1	
113	DFT study for the heterojunction effect in the precious metal clusters. *International Journal of Quantum Chemistry*, **2008**, 108, 2888-2895	2.1	3
112	Theoretical studies on effects of hydrogen bonds attaching to cysteine ligands on 4Fe-4S clusters. *International Journal of Quantum Chemistry*, **2008**, 108, 2881-2887	2.1	21
111	Theory of chemical bonds in metalloenzymes XI: Full geometry optimization and vibration analysis of porphyrin iron-oxo species. *International Journal of Quantum Chemistry*, **2008**, 108, 2950-2965	2.1	4
110	Theoretical studies on the structure and effective exchange integral (Jab) of an active site in oxyhemocyanin (oxyHc) by using approximately spin-projected geometry optimization (AP-opt) method. *Chemical Physics Letters*, **2008**, 456, 76-79	2.5	13
109	Theoretical investigation of the hetero-junction effect in PVP-stabilized Au13 clusters. The role of PVP in their catalytic activities. *Chemical Physics Letters*, **2008**, 459, 133-136	2.5	76
108	Approximately spin-projected geometry optimization method and its application to di-chromium systems. *Chemical Physics Letters*, **2007**, 442, 445-450	2.5	115
107	Assignments of the M□ssbauer spectra of an inorganic [8Fe□7S] complex based on the first-principle calculations. *Chemical Physics Letters*, **2007**, 446, 228-232	2.5	7
106	Theoretical studies of magnetic interaction of organic □radicals on gold cluster surface. *Polyhedron* , **2007**, 26, 2179-2182	2.7	3

105	Theoretical studies on ferromagnetic behavior of [Cr(C5(CH3)5)2]+[TCNE]□and [Mn(C5(CH3)5)2]+[TCNQ]□*Polyhedron*, **2007**, 26, 2135-2141	2.7	9
104	Theoretical studies on relation among structures, electric structures and magnetic interactions in MMX complexes. *Polyhedron*, **2007**, 26, 2154-2160	2.7	9
103	Theory of chemical bonds in metalloenzymes VI: Manganese□xo bonds in the photosynthesis II system. *Polyhedron*, **2007**, 26, 2216-2224	2.7	45
102	Ab initio studies on the zero-field splitting parameters of manganese porphyrin complexes. *Polyhedron*, **2007**, 26, 2309-2312	2.7	8
101	Theoretical studies of d□ magnetic interaction in organic superconductors. *Polyhedron*, **2007**, 26, 2304-2308	2.7	2
100	A GSO□IDFT study of noncollinear spin structures of [2Fe□S] cluster. *Polyhedron*, **2007**, 26, 2335-2341	2.7	2
99	Theoretical studies of radical spin arrangements in the cavity of nano-porous complexes. *Polyhedron*, **2007**, 26, 2367-2374	2.7	4
98	Theory of chemical bonds in metalloenzymes III: Full geometry optimization and vibration analysis of ferredoxin-type [2Fe□S] cluster. *International Journal of Quantum Chemistry*, **2007**, 107, 116-133	2.1	32
97	Theory of chemical bonds in metalloenzymes IV: Hybrid-DFT study of Rieske-type [2Fe?2S] clusters. *International Journal of Quantum Chemistry*, **2007**, 107, 609-627	2.1	29
96	Geometry optimization method based on approximate spin projection and its application to F2, CH2, CH2OO, and active site of urease. *International Journal of Quantum Chemistry*, **2007**, 107, 3094-3102	2.1	22
95	Theory of chemical bonds in metalloenzymes. IX. Theoretical study on the active site of the ribonucleotide reductase and the related species. *International Journal of Quantum Chemistry*, **2007**, 107, 3250-3265	2.1	12
94	Theory of chemical bonds in metalloenzymes. VII. Hybrid-density functional theory studies on the electronic structures of P450. *International Journal of Quantum Chemistry*, **2007**, 108, 631-650	2.1	17
93	Theoretical study of H2O and O2 adsorption on Au small clusters **2007**, 40, 40-44		41
92	Theoretical Study of the Change in the Magnetism and Conductivity of Diethylspirobiphenalenyl. *Chemistry Letters*, **2007**, 36, 1000-1001	1.7	2
91	Analytical TEM observation of Au nano-particles on cerium oxide. *Catalysis Today*, **2006**, 117, 62-68	5.3	78
90	Theoretical Calculations of Magnetic Interactions in Frustrated Antiferromagnetic Cluster. *Molecular Crystals and Liquid Crystals*, **2006**, 455, 135-141	0.5	1
89	N-band Hubbard models. III. Boson□ermion and interaction□oson models for high-Tc superconductivity. *International Journal of Quantum Chemistry*, **2006**, 106, 1052-1075	2.1	4
88	Theory of chemical bonds in metalloenzymes V: Hybrid-DFT studies of the inorganic [8Fe□S] core. *International Journal of Quantum Chemistry*, **2006**, 106, 3288-3302	2.1	28

87	DFT studies of interaction of Ir cluster with O2, CO and NO. *Catalysis Today*, **2006**, 111, 311-315	5.3	16
86	A hybrid density-functional study of the one-dimensional ferromagnetic ordering of (BDTA)[Ni(mnt)2]. *Chemical Physics Letters*, **2006**, 420, 397-400	2.5	
85	Hybrid-density functional study of magnetism and ligand control in Ni9 complexes. *Chemical Physics Letters*, **2006**, 421, 483-487	2.5	19
84	A general algorithm for calculation of Heisenberg exchange integrals J in multispin systems. *Chemical Physics Letters*, **2006**, 432, 343-347	2.5	219
83	Three-dimensional mesoporous titanosilicates prepared by modified sol-gel method: Ideal gold catalyst supports for enhanced propene epoxidation. *Journal of Physical Chemistry B*, **2005**, 109, 3956-65	3.4	97
82	A quantum chemical study of magnetic interactions in phenazine derivatives for chemical or photo-induced organic magnets. *Synthetic Metals*, **2005**, 154, 321-324	3.6	2
81	Theoretical studies of magnetic interaction in □radical thiol and Gold hybrid systems. *Synthetic Metals*, **2005**, 154, 313-316	3.6	6
80	Theoretical studies on magnetic interaction in one-dimensional CunBrm (S=1/2) chains. *Synthetic Metals*, **2005**, 154, 317-320	3.6	
79	Theoretical studies of magnetic interaction in organic □radical and gold cluster hybrid systems. *Polyhedron*, **2005**, 24, 2330-2336	2.7	7
78	Theoretical studies on dissociation of metal□arbon bond in Cobalamin: Formulation and calculation. *Polyhedron*, **2005**, 24, 2745-2750	2.7	1
77	Theoretical studies on magnetic interactions and charge-dope effects in one-dimensional Ni5 and Ni7 complexes. *Polyhedron*, **2005**, 24, 2751-2757	2.7	15
76	Possibilities of magnetic modifications of DNA wires, sheets and related materials. *Polyhedron*, **2005**, 24, 2758-2766	2.7	3
75	Theoretical studies on ferrimagnetic behavior of TCNE and manganese porphyrin dimer. *Polyhedron* , **2005**, 24, 2720-2725	2.7	14
74	A theoretical study of zero-field splitting of organic biradicals. *Polyhedron*, **2005**, 24, 2708-2715	2.7	35
73	Theoretical study on the magnetic interactions of active site in hemerythrin. *Polyhedron*, **2005**, 24, 2701-2707	2.7	14
72	Theoretical studies on magnetic interactions between Ni(II) ions in urease. *Polyhedron*, **2005**, 24, 2778-2783	2.7	4
71	Theoretical direct evaluation of inter-dimer J values in BETS salts. *Polyhedron*, **2005**, 24, 2382-2388	2.7	2
70	The interaction of neutral and charged Au clusters with O2, CO and H2. *Applied Catalysis A: General*, **2005**, 291, 37-44	5.1	93

69	Mechanistic insights in charge-transfer-induced luminescence of 1,2-dioxetanones with a substituent of low oxidation potential. *Journal of the American Chemical Society*, **2005**, 127, 8667-79	16.4	97
68	TEM observation of gold nanoparticles deposited on cerium oxide. *Journal of Materials Science*, **2005**, 40, 3101-3106	4.3	69
67	Search for the ground states of Ising spin clusters by using the genetic algorithms. *International Journal of Quantum Chemistry*, **2005**, 105, 645-654	2.1	4
66	Possibilities of molecule-based spintoronics of DNA wires, sheets, and related materials. *International Journal of Quantum Chemistry*, **2005**, 105, 655-671	2.1	9
65	Chemical bonding, less screening, and Hund's rule revisited. *International Journal of Quantum Chemistry*, **2005**, 105, 687-700	2.1	8
64	Quantum dynamics in high-spin molecules, spin dendrimers, and spin lattices. *International Journal of Quantum Chemistry*, **2005**, 105, 615-627	2.1	10
63	Theory of chemical bonds in metalloenzymes II: Hybrid-DFT studies in iron–sulfur clusters. *International Journal of Quantum Chemistry*, **2005**, 105, 628-644	2.1	24
62	Transmission electron microscopy observation of the structure of TiO2 nanotube and Au/TiO2 nanotube catalyst. *Surface and Interface Analysis*, **2005**, 37, 265-269	1.5	79
61	Theoretical studies on electronic states of Rh-C60. Possibility of a room-temperature organic ferromagnet. *Molecules*, **2004**, 9, 792-807	4.8	10
60	Local Barrier Height of Ir/TiO2Model Catalysts. *Japanese Journal of Applied Physics*, **2004**, 43, 4595-4598	1.4	5
59	Structural analyses by TEM of iridium deposited on TiO2 powder and rutile single crystal. *Journal of Electron Microscopy*, **2004**, 53, 29-35		7
58	Effect of Impurity and Pretreatment Conditions on the Catalytic Activity of Au Powder for CO Oxidation. *Catalysis Letters*, **2004**, 97, 203-208	2.8	54
57	Vapor-phase epoxidation of propylene using H2/O2 mixture over gold catalysts supported on non-porous and mesoporous titania-silica: effect of preparation conditions and pretreatments prior to reaction. *Applied Catalysis A: General*, **2004**, 263, 19-26	5.1	51
56	The electronic structure and magnetic property of metal-oxo, porphyrin manganese-oxo, and μ-oxo-bridged manganese porphyrin dimer. *International Journal of Quantum Chemistry*, **2004**, 100, 943-956	2.1	39
55	Theoretical studies on effective exchange integrals using spin correlation function analysis and magnetic effective density functional (MEDF) method. *International Journal of Quantum Chemistry*, **2004**, 100, 927-936	2.1	3
54	Theory of chemical bonds in metalloenzymes I: Analytical and hybrid-DFT studies on oxo and hydroxo diiron cores. *International Journal of Quantum Chemistry*, **2004**, 100, 887-906	2.1	48
53	Theoretical studies on magnetic interaction in one-dimensional spin chains of hydrogen atoms (Hn) and copper bromide (CunBrm). *International Journal of Quantum Chemistry*, **2004**, 100, 907-917	2.1	8
52	Vital role of moisture in the catalytic activity of supported gold nanoparticles. *Angewandte Chemie - International Edition*, **2004**, 43, 2129-32	16.4	525

51	Vital Role of Moisture in the Catalytic Activity of Supported Gold Nanoparticles. *Angewandte Chemie*, **2004**, 116, 2181-2184	3.6	70
50	Local barrier height of Au nanoparticles on a TiO2(1 1 0)-(1⁄2) surface. *Applied Surface Science*, **2004**, 222, 409-414	6.7	44
49	Electron holographic 3-D nano-analysis of Au/TiO2 catalyst at interface. *Journal of Electron Microscopy*, **2003**, 52, 21-6		28
48	Direct Production of Hydrogen Peroxide from H2and O2over Highly Dispersed Au catalysts. *Chemistry Letters*, **2003**, 32, 822-823	1.7	91
47	Multi-component noble metal catalysts prepared by sequential deposition precipitation for low temperature decomposition of dioxin. *Applied Catalysis B: Environmental*, **2003**, 41, 43-52	21.8	52
46	Preparation of supported gold catalysts by gas-phase grafting of gold acethylacetonate for low-temperature oxidation of CO and of H2. *Journal of Molecular Catalysis A*, **2003**, 199, 73-84		151
45	Effect of surface chemical properties and texture of mesoporous titanosilicates on direct vapor-phase epoxidation of propylene over Au catalysts at high reaction temperature. *Applied Catalysis A: General*, **2003**, 253, 75-89	5.1	57
44	Analytical TEM observation of Au and Ir deposited on rutile TiO2. *Journal of Electron Microscopy*, **2003**, 52, 119-24		30
43	Spin and Pseudo Spins in Theoretical Chemistry. A Unified View for Superposed and Entangled Quantum Systems. *Bulletin of the Korean Chemical Society*, **2003**, 24, 864-880	1.2	6
42	STM observations of organometallic complexes on the TiO2(1 1 0) and Si(1 1 1) surfaces. *Surface Science*, **2002**, 514, 267-272	1.8	9
41	Hydrogenation of 1,3-butadiene and of crotonaldehyde over highly dispersed Au catalysts. *Catalysis Today*, **2002**, 74, 265-269	5.3	190
40	CO Oxidation below Room Temperature over Ir/TiO2 Catalyst Prepared by Deposition Precipitation Method. *Journal of Catalysis*, **2002**, 208, 485-489	7.3	78
39	SEM and RHEEDREM Study of Au Particles Deposited on Rutile TiO2(110) by Deposition Precipitation and Gas-Phase Grafting Methods. *Journal of Catalysis*, **2002**, 212, 119-123	7.3	16
38	The influence of the support on the activity and selectivity of Pd in CO hydrogenation. *Applied Catalysis A: General*, **2001**, 213, 225-232	5.1	168
37	Influence of palladium precursors on methanol synthesis from CO hydrogenation over Pd/CeO2 catalysts prepared by depositionprecipitation method. *Applied Catalysis A: General*, **2001**, 217, 165-172	5.1	35
36	Effect of reduction temperature on structural properties and CO/CO2 hydrogenation characteristics of a Pd-CeO2 catalyst. *Applied Catalysis A: General*, **2001**, 217, 231-239	5.1	31
35	Epoxidation of propylene over gold catalysts supported on non-porous silica. *Applied Catalysis A: General*, **2001**, 218, 81-89	5.1	81
34	DFT studies of interaction between O 2 and Au clusters. The role of anionic surface Au atoms on Au clusters for catalyzed oxygenation. *Chemical Physics Letters*, **2001**, 346, 163-168	2.5	132

33	Low-Temperature Methanol Synthesis Catalyzed over Ultrafine Palladium Particles Supported on Cerium Oxide. *Journal of Catalysis*, **2001**, 197, 267-272	7.3	61
32	EPR Study of CO and O2 Interaction with Supported Au Catalysts. *Journal of Catalysis*, **2001**, 203, 168-174	7.3	106
31	Charge properties of red Argentine soils as an indicator of iron oxide/clay associations. *Soil Research*, **2001**, 39, 423	1.8	6
30	Surface properties of palladium supported on cerium oxide and its catalytic activity for methanol decomposition. *Studies in Surface Science and Catalysis*, **2000**, 130, 2315-2320	1.8	3
29	Preparation of Supported Gold Catalysts by Liquid-Phase Grafting of Gold Acethylacetonate for Low-Temperature Oxidation of CO and of H2. *Chemistry Letters*, **2000**, 29, 396-397	1.7	44
28	Surface Reducibility of Cerium Oxide Modified with Palladium. *Chemistry Letters*, **2000**, 29, 880-881	1.7	4
27	Effect of physical mixing of CsCl with Au/Ti-MCM-41 on the gas-phase epoxidation of propene using H2 and O2:. *Applied Catalysis A: General*, **2000**, 190, 43-50	5.1	87
26	C□SiC□Si gradient films formed on silicon by ion beam assisted deposition at room temperature. *Surface and Coatings Technology*, **2000**, 128-129, 274-279	4.4	4
25	Syntheses and EELS characterization of water-soluble multi-hydroxyl Gd@C82 fullerenols. *Chemical Physics Letters*, **2000**, 324, 255-259	2.5	49
24	Methanol synthesis from carbon monoxide and hydrogen catalyzed over Pd/CeO2 prepared by the deposition□precipitation method. *Catalysis Letters*, **2000**, 64, 23-25	2.8	50
23	Theoretical Studies of the Pressure Effects for □Phase of p-NPNN. *Molecular Crystals and Liquid Crystals*, **1999**, 335, 623-632		3
22	Exchange interactions in the genuine organic ferromagnet accompanying pressure-induced ferro- to antiferromagnetic transition. *Chemical Physics Letters*, **1999**, 308, 181-186	2.5	15
21	Low-temperature Methanol Synthesis Catalyzed over Pd/CeO2. *Chemistry Letters*, **1999**, 28, 1101-1102	1.7	4
20	No participation of adenosine A1 receptor in acute nephrotoxicity by 4-pentenoic acid administration in dogs. *The Japanese Journal of Pharmacology*, **1999**, 80, 223-8		
19	Chemical vapor deposition of gold on Al2O3, SiO2, and TiO2 for the oxidation of CO and of H2. *Catalysis Letters*, **1998**, 51, 53-58	2.8	407
18	Deposition of gold nanoparticles on silica by CVD of gold acethylacetonate. *Studies in Surface Science and Catalysis*, **1998**, 118, 277-284	1.8	14
17	Chemical Vapor Deposition of Gold Nanoparticles on MCM-41 and Their Catalytic Activities for the Low-temperature Oxidation of CO and of H2. *Chemistry Letters*, **1998**, 27, 315-316	1.7	110
16	Low-temperature decomposition of methanol to carbon monoxide and hydrogen with low activation energy over Pd/ZrO2 catalyst. *Catalysis Letters*, **1997**, 44, 189-191	2.8	75

15	The reactivities of dimethylgold(III)□diketone on the surface of TiO2 A novel preparation method for Au catalysts. *Solid State Ionics*, **1997**, 95, 143-149	3.3	109
14	CASSCF and CASPT2 calculations of hole-doped amines with triplet carbene groups. Possibilities of high-Tc organic ferrimagnets. *Chemical Physics Letters*, **1995**, 233, 88-94	2.5	30
13	CASSCF and CASPT2 calculations of hole-doped polycarbenes. Possibilities of organic ferromagnetic conductors and metals. *Chemical Physics Letters*, **1995**, 233, 257-265	2.5	52
12	A MO-theoretical calculation of the antiferromagnetism in the □phase of p-nitrophenyl nitronyl nitroxide. *Chemical Physics Letters*, **1994**, 219, 36-44	2.5	27
11	CASPT2 and MR MP2 calculations of potential curves and effective exchange integrals for the dimer of triplet methylene. *Chemical Physics Letters*, **1994**, 225, 213-220	2.5	39
10	Electronic structures of poly-cations and -anions of C60. Possible mechanisms of organic ferromagnetism. *Chemical Physics Letters*, **1994**, 226, 372-380	2.5	39
9	Ferromagnetic intermolecular interaction of the cation radical ofm-N-methylpyridinium nitronyl nitroxide. A CASSCF study. *Chemical Physics Letters*, **1994**, 228, 575-582	2.5	16
8	Theoretical Studies of Magnetic Orderings in the □and □Phases of P-NPNN and Related Nitroxides. *Molecular Crystals and Liquid Crystals*, **1993**, 232, 35-44		24
7	A theoretical explanation of the organic ferromagnetism in the □phase of para-nitrophenyl nitronyl nitroxide. *Chemical Physics Letters*, **1993**, 207, 1-8	2.5	39
6	High-spin ion radicals of polyenes and polyamines. A MO theoretical study. *Chemical Physics Letters*, **1993**, 207, 9-14	2.5	28
5	Comparison between spin restricted and unrestricted post-Hartree□ock calculations of effective exchange integrals in Ising and Heisenberg models. *Chemical Physics Letters*, **1993**, 210, 201-210	2.5	81
4	Mechanical properties and microstructures of machinable silicon carbide. *Journal of Materials Science*, **1993**, 28, 1175-1181	4.3	25
3	MO theoretical studies of magnetic interactions in clusters of nitronyl nitroxide and related species. *Chemical Physics Letters*, **1992**, 190, 353-360	2.5	68
2	New models for organic magnetic conductors or organic kondo and dense kondo systems. *Synthetic Metals*, **1991**, 43, 3631-3634	3.6	47
1	CNDO/S-CI Calculations of Hyperpolarizabilities. III. Regular Polyenes, Charged Polyenes, Di-substituted Polyenes, Polydiacetylene and Related Species. *Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics*, **1990**, 182, 1-15		8