Mitsutaka Okumura

List of Publications by Citations

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	Vital role of moisture in the catalytic activity of supported gold nanoparticles. *Angewandte Chemie - International Edition*, **2004**, 43, 2129-32	16.4	525
319	Catalytically highly active top gold atom on palladium nanocluster. *Nature Materials*, **2011**, 11, 49-52	27	486
318	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
317	Hydrogen dissociation by gold clusters. *Angewandte Chemie - International Edition*, **2009**, 48, 9515-8	16.4	253
316	A general algorithm for calculation of Heisenberg exchange integrals J in multispin systems. *Chemical Physics Letters*, **2006**, 432, 343-347	2.5	219
315	Hydrogenation of 1,3-butadiene and of crotonaldehyde over highly dispersed Au catalysts. *Catalysis Today*, **2002**, 74, 265-269	5.3	190
314	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
313	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
312	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
311	Approximately spin-projected geometry optimization method and its application to di-chromium systems. *Chemical Physics Letters*, **2007**, 442, 445-450	2.5	115
310	Heterogeneous Catalysis by Gold. *Advances in Catalysis*, **2012**, 55, 1-126	2.4	113
309	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
308	The reactivities of dimethylgold(III)β-diketone on the surface of TiO2 A novel preparation method for Au catalysts. *Solid State Ionics*, **1997**, 95, 143-149	3.3	109
307	EPR Study of CO and O2 Interaction with Supported Au Catalysts. *Journal of Catalysis*, **2001**, 203, 168-174	4.3	106
306	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
305	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
304	The interaction of neutral and charged Au clusters with O2, CO and H2. *Applied Catalysis A: General*, **2005**, 291, 37-44	5.1	93

303	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
302	Direct Production of Hydrogen Peroxide from H2and O2over Highly Dispersed Au catalysts. *Chemistry Letters*, **2003**, 32, 822-823	1.7	91
301	MicroRNA-mediated downregulation of mTOR/FGFR3 controls tumor growth induced by Src-related oncogenic pathways. *Oncogene*, **2011**, 30, 3489-501	9.2	87
300	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
299	Epoxidation of propylene over gold catalysts supported on non-porous silica. *Applied Catalysis A: General*, **2001**, 218, 81-89	5.1	81
298	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
297	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
296	Analytical TEM observation of Au nano-particles on cerium oxide. *Catalysis Today*, **2006**, 117, 62-68	5.3	78
295	CO Oxidation below Room Temperature over Ir/TiO2 Catalyst Prepared by Deposition Precipitation Method. *Journal of Catalysis*, **2002**, 208, 485-489	7.3	78
294	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
293	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
292	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
291	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
290	Vital Role of Moisture in the Catalytic Activity of Supported Gold Nanoparticles. *Angewandte Chemie*, **2004**, 116, 2181-2184	3.6	70
289	TEM observation of gold nanoparticles deposited on cerium oxide. *Journal of Materials Science*, **2005**, 40, 3101-3106	4.3	69
288	MO theoretical studies of magnetic interactions in clusters of nitronyl nitroxide and related species. *Chemical Physics Letters*, **1992**, 190, 353-360	2.5	68
287	Possible mechanisms of water splitting reaction based on proton and electron release pathways revealed for CaMn4O5 cluster of PSII refined to 1.9 X-ray resolution. *International Journal of Quantum Chemistry*, **2012**, 112, 253-276	2.1	63
286	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

285	An extremely bright heteroleptic bis(dipyrrinato)zinc(II) complex. *Chemistry - an Asian Journal*, **2012**, 7, 907-10	4.5	61
284	Low-Temperature Methanol Synthesis Catalyzed over Ultrafine Palladium Particles Supported on Cerium Oxide. *Journal of Catalysis*, **2001**, 197, 267-272	7.3	61
283	A Career in Catalysis: Masatake Haruta. *ACS Catalysis*, **2015**, 5, 4699-4707	13.1	60
282	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
281	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
280	Transition state optimization based on approximate spin-projection (AP) method. *Chemical Physics Letters*, **2009**, 483, 168-171	2.5	58
279	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
278	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
277	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
276	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
275	Hydrogen Dissociation by Gold Clusters. *Angewandte Chemie*, **2009**, 121, 9679-9682	3.6	53
274	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
273	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
272	Colloidal Au single-atom catalysts embedded on Pd nanoclusters. *Journal of Materials Chemistry A*, **2014**, 2, 13498-13508	13	51
271	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
270	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
269	Syntheses and EELS characterization of water-soluble multi-hydroxyl Gd@C82 fullerenols. *Chemical Physics Letters*, **2000**, 324, 255-259	2.5	49
268	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

267	New models for organic magnetic conductors or organic kondo and dense kondo systems. *Synthetic Metals*, **1991**, 43, 3631-3634	3.6	47
266	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
265	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
264	Theory of chemical bonds in metalloenzymes VI: Manganese□xo bonds in the photosynthesis II system. *Polyhedron*, **2007**, 26, 2216-2224	2.7	45
263	Local barrier height of Au nanoparticles on a TiO2(1 1 0)-(1□) surface. *Applied Surface Science*, **2004**, 222, 409-414	6.7	44
262	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
261	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
260	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
259	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
258	Advances in Gold Catalysis and Understanding the Catalytic Mechanism. *Chemical Record*, **2016**, 16, 2278-2293	6.6	41
257	Theoretical study of H2O and O2 adsorption on Au small clusters **2007**, 40, 40-44		41
256	Crown Jewel catalyst: How neighboring atoms affect the catalytic activity of top Au atoms?. *Journal of Catalysis*, **2013**, 305, 7-18	7.3	40
255	Extraordinary Aggregation of Inorganic Anions in Chiral Metallosupramolecular Ionic Crystals. *Bulletin of the Chemical Society of Japan*, **2013**, 86, 908-920	5.1	39
254	The electronic structure and magnetic property of metal-oxo, porphyrin manganese-oxo, and □xo-bridged manganese porphyrin dimer. *International Journal of Quantum Chemistry*, **2004**, 100, 943-956	2.1	39
253	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
252	Electronic structures of poly-cations and -anions of C60. Possible mechanisms of organic ferromagnetism. *Chemical Physics Letters*, **1994**, 226, 372-380	2.5	39
251	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
250	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

249	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
248	Synthesis and catalytic activity of crown jewel-structured (IrPd)/Au trimetallic nanoclusters. *Advanced Materials*, **2015**, 27, 1383-8	24	35
247	A theoretical study of zero-field splitting of organic biradicals. *Polyhedron*, **2005**, 24, 2708-2715	2.7	35
246	Influence of palladium precursors on methanol synthesis from CO hydrogenation over Pd/CeO2 catalysts prepared by deposition precipitation method. *Applied Catalysis A: General*, **2001**, 217, 165-172	5.1	35
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	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
243	Theory of chemical bonds in metalloenzymes III: Full geometry optimization and vibration analysis of ferredoxin-type [2Fe2S] cluster. *International Journal of Quantum Chemistry*, **2007**, 107, 116-133	2.1	32
242	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
241	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
240	Electronic and Spin Structures of the CaMn4O5(H2O)4 Cluster in OEC of PSII Refined to 1.9 X-ray Resolution. *Advances in Quantum Chemistry*, **2012**, 64, 121-187	1.4	30
239	Consistent scheme for computing standard hydrogen electrode and redox potentials. *Journal of Computational Chemistry*, **2013**, 34, 21-6	3.5	30
238	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
237	Analytical TEM observation of Au and Ir deposited on rutile TiO2. *Journal of Electron Microscopy*, **2003**, 52, 119-24		30
236	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
235	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
234	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
233	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
232	Theory of chemical bonds in metalloenzymes V: Hybrid-DFT studies of the inorganic [8Fe7S] core. *International Journal of Quantum Chemistry*, **2006**, 106, 3288-3302	2.1	28

231	Electron holographic 3-D nano-analysis of Au/TiO2 catalyst at interface. *Journal of Electron Microscopy*, **2003**, 52, 21-6		28
230	High-spin ion radicals of polyenes and polyamines. A MO theoretical study. *Chemical Physics Letters*, **1993**, 207, 9-14	2.5	28
229	Asymmetric dinuclear bis(dipyrrinato)zinc(II) complexes: broad absorption and unidirectional quantitative exciton transmission. *Chemical Communications*, **2014**, 50, 5881-3	5.8	27
228	A MO-theoretical calculation of the antiferromagnetism in the β-phase of p-nitrophenyl nitronyl nitroxide. *Chemical Physics Letters*, **1994**, 219, 36-44	2.5	27
227	Fluorescent azadipyrrinato zinc(II) complex: hybridisation with a dipyrrinato ligand. *Dalton Transactions*, **2012**, 41, 14035-7	4.3	25
226	Mechanical properties and microstructures of machinable silicon carbide. *Journal of Materials Science*, **1993**, 28, 1175-1181	4.3	25
225	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
224	Theoretical Studies of Magnetic Orderings in the α- and β-Phases of P-NPNN and Related Nitroxides. *Molecular Crystals and Liquid Crystals*, **1993**, 232, 35-44		24
223	Unique structural and electronic features of perferryl-oxo oxidant in Cytochrome P450. *Journal of Physical Chemistry B*, **2011**, 115, 10730-8	3.4	23
222	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
221	π-Conjugated trinuclear group-9 metalladithiolenes with a triphenylene backbone. *Inorganic Chemistry*, **2013**, 52, 7411-6	5.1	22
220	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
219	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
218	meso-Alkynyl BODIPYs: structure, photoproperties, π-extension, and manipulation of frontier orbitals. *Chemistry - an Asian Journal*, **2013**, 8, 723-7	4.5	21
217	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
216	Interplay of theoretical calculations and experiments for a study of catalysis by gold. *Catalysis Today*, **2016**, 259, 81-86	5.3	20
215	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
214	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

213	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
212	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
211	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
210	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
209	Diffuse Unoccupied Molecular Orbital of Rubrene Causing Image-Potential State Mediated Excitation. *Journal of Physical Chemistry C*, **2013**, 117, 20098-20103	3.8	19
208	Hybrid-density functional study of magnetism and ligand control in Ni9 complexes. *Chemical Physics Letters*, **2006**, 421, 483-487	2.5	19
207	Effect of spin contamination error on surface catalytic reaction: NO reduction by core-shell catalysts. *Molecular Physics*, **2019**, 117, 2251-2259	1.7	18
206	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
205	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
204	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
203	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
202	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
201	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
200	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
199	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
198	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
197	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
196	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

195	Ab initio study of magnetic interactions of manganese-oxide clusters. *Polyhedron*, **2011**, 30, 3256-3261	2.7	16
194	DFT studies of interaction of Ir cluster with O2, CO and NO. *Catalysis Today*, **2006**, 111, 311-315	5.3	16
193	SEM and RHEED–REM 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
192	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
191	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
190	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
189	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
188	Hydrogen Production from Water Using Novel Three-dimensional Interpenetrated Zn–Pd Coordination Polymer. *Chemistry Letters*, **2010**, 39, 878-880	1.7	15
187	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
186	Theoretical studies on magnetic interactions and charge-dope effects in one-dimensional Ni5 and Ni7 complexes. *Polyhedron*, **2005**, 24, 2751-2757	2.7	15
185	Exchange interactions in the genuine organic ferromagnet accompanying pressure-induced ferro- to antiferromagnetic transition. *Chemical Physics Letters*, **1999**, 308, 181-186	2.5	15
184	Crystalline-Amorphous-Crystalline Transformation in a Highly Brilliant Luminescent System with Trigonal-Planar Gold(I) Centers. *Scientific Reports*, **2016**, 6, 26002	4.9	15
183	Potential of Titania-covered Ag Catalysts for NOx Reduction: A DFT Study. *Chemistry Letters*, **2017**, 46, 456-459	1.7	14
182	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
181	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
180	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
179	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
178	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

177	Theoretical studies on ferrimagnetic behavior of TCNE and manganese porphyrin dimer. *Polyhedron*, **2005**, 24, 2720-2725	2.7	14
176	Theoretical study on the magnetic interactions of active site in hemerythrin. *Polyhedron*, **2005**, 24, 2701-2707	2.7	14
175	Deposition of gold nanoparticles on silica by CVD of gold acethylacetonate. *Studies in Surface Science and Catalysis*, **1998**, 118, 277-284	1.8	14
174	Computational Study of Catalytic Reaction of Quercetin 2,4-Dioxygenase. *Journal of Physical Chemistry B*, **2015**, 119, 6952-62	3.4	13
173	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
172	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
171	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
170	DFT and DFT-D studies on molecular structure of double-decker phthalocyaninato-terbium(III) complex. *Molecular Physics*, **2014**, 112, 995-1001	1.7	13
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165	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
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