Masahiro Ehara

List of Publications by Year in Descending Order

251 papers	5,359 citations	38 h-index	56 g-index
278 ext. papers	5,912 ext. citations	4.2 avg, IF	5.86 L-index

#	Paper	IF	Citations
251	Asymmetric Twisting of -Centered Octahedral Gold(I) Clusters by Chiral -Heterocyclic Carbene Ligation.. *Journal of the American Chemical Society*, **2022**,	16.4	2
250	Theoretical Study of the Propene Combustion Catalysis of Chromite Spinels: Reaction Mechanism and Relation between the Activity and Electronic Structure of Spinels. *Journal of Physical Chemistry C*, **2021**, 125, 25983-26002	3.8	0
249	Lifetimes of Be and Mg Cluster Dianions. *Journal of Physical Chemistry A*, **2021**, 125, 3579-3588	2.8	3
248	Attenuated Total Reflection-Far-Ultraviolet Spectroscopy and Quantum Chemical Calculations of the Electronic Structure of the Top Surface and Bulk of Polyethylenes with Different Crystallinities. *Applied Spectroscopy*, **2021**, 75, 971-979	3.1	2
247	Catalytic Oxidation of Benzyl Alcohol to Benzaldehyde on Au8 and Au6Pd2 Clusters: A DFT Study on the Reaction Mechanism. *Catalysts*, **2021**, 11, 720	4	0
246	Mechanistic Studies on Photoinduced Catalytic Olefin Migration Reactions at the Pd(II) Centers of a Porous Crystal, Metal-Macrocycle Framework. *Chemistry - an Asian Journal*, **2021**, 16, 202-206	4.5	2
245	Theoretical insight into oxidation catalysis of chromite spinel MCr2O4 (M□=□Mg, Co, Cu, and Zn): Volcano plot for oxygen-vacancy formation and catalytic activity. *Journal of Catalysis*, **2021**, 393, 30-41	7.3	6
244	The emergence of intense near-infrared photoluminescence by photoactivation of silver nanoclusters. *Chemical Communications*, **2021**, 57, 6483-6486	5.8	0
243	Selective catalytic reduction of NO with NH3 over Cu-exchanged CHA, GME, and AFX zeolites: a density functional theory study. *Catalysis Science and Technology*, **2021**, 11, 1780-1790	5.5	6
242	AFX Zeolite for Use as a Support of NH3-SCR Catalyst Mining through AICE Joint Research Project of Industries□Academia□Academia. *Catalysts*, **2021**, 11, 163	4	2
241	A comparative study of [Ag(PrS)(dppb)] and [AgS(BuS)(dppb)]: templating effect on structure and photoluminescence. *Dalton Transactions*, **2021**, 50, 10561-10566	4.3	0
240	Stabilities, Electronic Structures, and Bonding Properties of 20-Electron Transition Metal Complexes (Cp)TMO and their One-Dimensional Sandwich Molecular Wires (Cp = CH, C(CH)H, C(CH); TM = Cr, Mo, W). *Journal of Physical Chemistry A*, **2021**, 125, 721-730	2.8	1
239	Oxidation and Storage Mechanisms for Nitrogen Oxides on Variously Terminated (001) Surfaces of SrFeO and SrFeO Perovskites. *ACS Applied Materials & Interfaces*, **2021**, 13, 7216-7226	9.5	6
238	Theoretical Study of NO Dissociative Adsorption onto 3d Metal Particles M (M = Fe, Co, Ni, and Cu): Relation between the Reactivity and Position of the Metal Element in the Periodic Table. *ACS Omega*, **2021**, 6, 4888-4898	3.9	2
237	Facet-dependent catalytic activity of anatase TiO2 for the selective catalytic reduction of NO with NH3: A dispersion-corrected density functional theory study. *Applied Catalysis A: General*, **2021**, 623, 118250	5.1	0
236	Origin of the Aggregation-Induced Phosphorescence of Platinum(II) Complexes: The Role of Metal-Metal Interactions on Emission Decay in the Crystalline State. *Chemistry - an Asian Journal*, **2021**, 16, 3129-3140	4.5	1
235	Substitution effect on the nonradiative decay and -iphotoisomerization route: a guideline to develop efficient cinnamate-based sunscreens. *Physical Chemistry Chemical Physics*, **2021**, 23, 834-845	3.6	3

234	Lithium–Bromine exchange reaction on C60: first theoretical proposal of a stable singlet fullerene carbene without the heteroatom. *Organic Chemistry Frontiers*, **2021**, 8, 1551-1562	5.2	0
233	Covalent interactions depend on the distances between metals and fullerenes for thermodynamically stable M@C78 (M = La, Ce, and Sm). *Inorganic Chemistry Frontiers*, **2020**, 7, 2538-2547	6.8	3
232	Impact of Enantiomeric Ligand Composition on the Photophysical Properties of Chiral Ag29 Nanoclusters. *Bulletin of the Chemical Society of Japan*, **2020**, 93, 834-840	5.1	1
231	Theoretical Design of Photofunctional Molecular Aggregates for Optical Properties: An Inverse Design Approach. *Journal of Physical Chemistry C*, **2020**, 124, 13329-13337	3.8	4
230	Pt-Pd Nanoalloy for the Unprecedented Activation of Carbon-Fluorine Bond at Low Temperature. *Bulletin of the Chemical Society of Japan*, **2020**, 93, 1180-1185	5.1	2
229	Propene oxidation catalysis and electronic structure of M particles (M = Pd or Rh): differences and similarities between Pd and Rh. *Physical Chemistry Chemical Physics*, **2020**, 22, 11783-11796	3.6	5
228	Potential molecular semiconductor devices: cyclo-C (n = 10 and 14) with higher stabilities and aromaticities than acknowledged cyclo-C. *Physical Chemistry Chemical Physics*, **2020**, 22, 4823-4831	3.6	16
227	Combination of a Voronoi-Type Complex Absorbing Potential with the XMS-CASPT2 Method and Pilot Applications. *Journal of Chemical Theory and Computation*, **2020**, 16, 2606-2616	6.4	8
226	DFT/TD-DFT investigation on the photoinduced electron transfer of diruthenium and viologen complexes. *Journal of Luminescence*, **2020**, 222, 117121	3.8	2
225	Time-Dependent Density Functional Theory Investigation of Excited State Intramolecular Proton Transfer in Tris(2-hydroxyphenyl)triazasumanene. *Journal of Physical Chemistry A*, **2020**, 124, 1227-1234	2.8	5
224	Enantioseparation and chiral induction in Ag nanoclusters with intrinsic chirality. *Chemical Science*, **2020**, 11, 2394-2400	9.4	18
223	Crystallographic Characterization of ErC@C: Cluster Stretching with Cage Elongation. *Inorganic Chemistry*, **2020**, 59, 1940-1946	5.1	11
222	Importance of the Pd and Surrounding Sites in Hydrosilylation of Internal Alkynes by Palladium–Gold Alloy Catalyst. *Organometallics*, **2020**, 39, 528-537	3.8	7
221	Reaction mechanism, norbornene and ligand effects, and origins of meta-selectivity of Pd/norbornene-catalyzed C–H activation. *Chemical Science*, **2020**, 11, 113-125	9.4	8
220	Theoretical Investigation of the Key Roles in Fullerene-Formation Mechanisms: Enantiomer and Enthalpy. *ACS Applied Nano Materials*, **2020**, 3, 547-554	5.6	6
219	Theoretical study on 31P NMR chemical shifts of phosphorus-modified CHA zeolites. *Microporous and Mesoporous Materials*, **2020**, 294, 109908	5.3	20
218	Resonant states in cyanogen NCCN. *Physical Chemistry Chemical Physics*, **2020**, 22, 23141-23147	3.6	4
217	Stabilities, Electronic Structures, and Bonding Properties of Iron Complexes (EE)Fe(CO)(CNAr) (EE=BF, CO, N, CN, or NO). *ChemistryOpen*, **2020**, 9, 1195-1201	2.3	2

216	Deep learning enabled inorganic material generator. *Physical Chemistry Chemical Physics*, **2020**, 22, 26935-26943	3.6	31
215	Theoretical Insight into Thermodynamically Optimal U@C: Three-Electron Transfer Rather Than Four-Electron Transfer. *Inorganic Chemistry*, **2020**, 59, 12650-12658	5.1	2
214	Crystallographic characterization of ErC@C(43)-C, ErC@C(40)-C, ErC@C(44)-C, and ErC@C(21)-C: the role of cage-shape on cluster configuration. *Nanoscale*, **2019**, 11, 17319-17326	7.7	20
213	Pivotal Role of Nonmetal Atoms in the Stabilities, Geometries, Electronic Structures, and Isoelectronic Chemistry of Sc X@C (X = C, N, and O). *Journal of Computational Chemistry*, **2019**, 40, 2730-2738	3.5	9
212	Gold-Palladium Nanocluster Catalysts for Homocoupling: Electronic Structure and Interface Dynamics. *Chemical Record*, **2019**, 19, 947-959	6.6	8
211	Crystallographic characterization of ErN@C (2n = 80, 82, 84, 88): the importance of a planar ErN cluster. *Nanoscale*, **2019**, 11, 13415-13422	7.7	10
210	The direct observation of the doorway n□ state of methylcinnamate and hydrogen-bonding effects on the photochemistry of cinnamate-based sunscreens. *Physical Chemistry Chemical Physics*, **2019**, 21, 19755-19763	3.6	12
209	Light-driven molecular switch for reconfigurable spin filters. *Nature Communications*, **2019**, 10, 2455	17.4	68
208	Influence of local strain caused by cycloaddition on the band gap control of functionalized single-walled carbon nanotubes.. *RSC Advances*, **2019**, 9, 13998-14003	3.7	14
207	Theoretical and Experimental Molecular Spectroscopy of the Far-Ultraviolet Region **2019**, 119-145		4
206	Theoretical Study on the Optical Properties of Multichromophoric Systems Based on an Exciton Approach: Modification Guidelines. *ChemPhotoChem*, **2019**, 3, 707-718	3.3	2
205	Mechanistic insight into the catalytic hydrogenation of nonactivated aldehydes with a Hantzsch ester in the presence of a series of organoboranes: NMR and DFT studies.. *RSC Advances*, **2019**, 9, 10201-10210	3.7	5
204	High Turnover Frequency CO□NO Reactions over Rh Overlayer Catalysts: A Comparative Study Using Rh Nanoparticles. *Journal of Physical Chemistry C*, **2019**, 123, 6080-6089	3.8	12
203	Catalysis of Cu Cluster for NO Reduction by CO: Theoretical Insight into the Reaction Mechanism. *ACS Omega*, **2019**, 4, 2596-2609	3.9	21
202	Photophysical properties of fluorescent imaging biological probes of nucleic acids: SAC-CI and TD-DFT Study. *Journal of Computational Chemistry*, **2019**, 40, 127-134	3.5	3
201	In-Depth Theoretical Probe into Novel Mixed-Metal Uranium-Based Endohedral Clusterfullerenes ScUX@(31924)-C (X = C, N). *Inorganic Chemistry*, **2019**, 58, 10769-10777	5.1	9
200	Reaction Behavior of the NO Molecule on the Surface of an M Particle (M = Ru, Rh, Pd, and Ag; = 13 and 55): Theoretical Study of Its Dependence on Transition-Metal Element. *Journal of Physical Chemistry A*, **2019**, 123, 7021-7033	2.8	15
199	Theoretical Insight into Configurational Selectivity of Functionalized Single-Walled Carbon Nanotubes Based on the Clar Sextet Theory. *Journal of Physical Chemistry C*, **2019**, 123, 18629-18637	3.8	2

198	New Insight into U@C: Missing U@(31921)-C and Nuanced Enantiomers of U@(28324)-C. *Inorganic Chemistry*, **2019**, 58, 14159-14166	5.1	11
197	Theoretical Study on the Optical Properties of Multichromophoric Systems Based on an Exciton Approach: Modification Guidelines. *ChemPhotoChem*, **2019**, 3, 663-663	3.3	
196	Thermodynamic control of quantum defects on single-walled carbon nanotubes. *Chemical Communications*, **2019**, 55, 13757-13760	5.8	5
195	Enhanced oxygen reduction activity of platinum subnanocluster catalysts through charge redistribution. *Chemical Communications*, **2019**, 55, 12603-12606	5.8	10
194	Lewis Acid Catalysis of Nb2O5 for Reactions of Carboxylic Acid Derivatives in the Presence of Basic Inhibitors. *ChemCatChem*, **2019**, 11, 383-396	5.2	30
193	Heat-Resistant Properties in the Phosphorescence of trans-Bis[(iminomethyl)aryloxy]platinum(II) Complexes: Effect of Aromaticity on d-Conjugation Platforms. *Chemistry - A European Journal*, **2019**, 25, 3650-3661	4.8	10
192	Electronic processes in NO dimerization on Ag and Cu clusters: DFT and MRMP2 studies. *Journal of Computational Chemistry*, **2019**, 40, 181-190	3.5	6
191	ESIPT emission behavior of methoxy-substituted 2-hydroxyphenylbenzimidazole isomers. *New Journal of Chemistry*, **2018**, 42, 5923-5928	3.6	16
190	Theoretical Insights into Monometallofullerene Th@C: Strong Covalent Interaction between Thorium and the Carbon Cage. *Inorganic Chemistry*, **2018**, 57, 2961-2964	5.1	17
189	Different photoisomerization routes found in the structural isomers of hydroxy methylcinnamate. *Physical Chemistry Chemical Physics*, **2018**, 20, 17583-17598	3.6	16
188	Frenkel-exciton decomposition analysis of circular dichroism and circularly polarized luminescence for multichromophoric systems. *Journal of Computational Chemistry*, **2018**, 39, 931-935	3.5	7
187	Temporary Anion States of Ethene Interacting with Single Molecules of Methane, Ethane, and Water. *Journal of Physical Chemistry A*, **2018**, 122, 2580-2586	2.8	3
186	Nickel-catalyzed coupling reaction of alkyl halides with aryl Grignard reagents in the presence of 1,3-butadiene: mechanistic studies of four-component coupling and competing cross-coupling reactions. *Chemical Science*, **2018**, 9, 2195-2211	9.4	31
185	Origin of Nb O Lewis Acid Catalysis for Activation of Carboxylic Acids in the Presence of a Hard Base. *ChemPhysChem*, **2018**, 19, 2848-2857	3.2	19
184	Ni-Catalyzed Dimerization and Hydroperfluoroarylation of 1,3-Dienes. *Journal of Organic Chemistry*, **2018**, 83, 9267-9277	4.2	13
183	Silicon-coordinated nitrogen-doped graphene as a promising metal-free catalyst for NO reduction by CO: a theoretical study.. *RSC Advances*, **2018**, 8, 22322-22330	3.7	19
182	Control of near infrared photoluminescence properties of single-walled carbon nanotubes by functionalization with dendrons. *Nanoscale*, **2018**, 10, 23012-23017	7.7	10
181	Preferential Photoreaction in a Porous Crystal, Metal-Macrocycle Framework: Pd-Mediated Olefin Migration over [2+2] Cycloaddition. *Journal of the American Chemical Society*, **2018**, 140, 16610-16614	16.4	19

180	Origin of Nb2O5 Lewis Acid Catalysis for Activation of Carboxylic Acids in the Presence of a Hard Base. *ChemPhysChem*, **2018**, 19, 2809-2809	3.2	
179	Mechanism of NO□CO reaction over highly dispersed cuprous oxide on □alumina catalyst using a metal□support interfacial site in the presence of oxygen: similarities to and differences from biological systems. *Catalysis Science and Technology*, **2018**, 8, 3833-3845	5.5	9
178	Computational Studies on Reaction Mechanism and Origins of Selectivities in Nickel-Catalyzed (2 + 2 + 2) Cycloadditions and Alkenylative Cyclizations of 1,6-Ene-Allenes and Alkenes. *Journal of Organic Chemistry*, **2017**, 82, 2150-2159	4.2	10
177	A Theoretical Investigation on CO Oxidation by Single-Atom Catalysts M/□AlO (M=Pd, Fe, Co, and Ni). *ChemCatChem*, **2017**, 9, 1222-1229	5.2	63
176	Changes in the Electronic States of Low-Temperature Solid -Tetradecane: Decrease in the HOMO-LUMO Gap. *ACS Omega*, **2017**, 2, 618-625	3.9	20
175	Probing the electronic structures of Co (n = 1-5) clusters on □AlO surfaces using first-principles calculations. *Physical Chemistry Chemical Physics*, **2017**, 19, 3679-3687	3.6	14
174	Comparing the performance of TD-DFT and SAC-CI methods in the description of excited states potential energy surfaces: An excited state proton transfer reaction as case study. *Journal of Computational Chemistry*, **2017**, 38, 1084-1092	3.5	13
173	Resonance Energies and Lifetimes from the Analytic Continuation of the Coupling Constant Method: Robust Algorithms and a Critical Analysis. *Journal of Chemical Theory and Computation*, **2017**, 13, 2550-2560	6.4	7
172	Core□Shell versus Other Structures in Binary Cu38□Mn Nanoclusters (M = Ru, Rh, Pd, Ag, Os, Ir, Pt, and Au; n = 1, 2, and 6): Theoretical Insight into Determining Factors. *Journal of Physical Chemistry C* , **2017**, 121, 10514-10528	3.8	16
171	Diels-Alder Cycloaddition of Cyclopentadiene and C at the Extreme High Pressure. *Journal of Physical Chemistry A*, **2017**, 121, 4363-4371	2.8	12
170	Structures of Bimetallic Copper□Ruthenium Nanoparticles: Incoherent Interface and Surface Active Sites for Catalytic Nitric Oxide Dissociation. *Journal of Physical Chemistry C*, **2017**, 121, 300-307	3.8	11
169	Synthesis and Optical Properties of Excited-State Intramolecular Proton Transfer Active □Conjugated Benzimidazole Compounds: Influence of Structural Rigidification by Ring Fusion. *Journal of Organic Chemistry*, **2017**, 82, 12173-12180	4.2	23
168	Theoretical Insight into ScC: Carbide Clusterfullerene ScC@C versus Dimetallofullerene Sc@C. *Inorganic Chemistry*, **2017**, 56, 10195-10203	5.1	11
167	Deciphering the Role of Long-Range Interaction in Endohedral Metallofullerenes: A Revisit to Sc2C70. *Journal of Physical Chemistry C*, **2017**, 121, 20481-20488	3.8	4
166	Quantum Chemical Insight into LaC: Metal Carbide Fullerene LaC@C versus Dimetallofullerene La@C. *Inorganic Chemistry*, **2017**, 56, 11883-11890	5.1	8
165	Intramolecular Hydroamination by a Primary Amine of an Unactivated Alkene on Gold Nanoclusters: A DFT Study. *ChemCatChem*, **2017**, 9, 4490-4500	5.2	6
164	Synthesis and Optical Properties of Fused □Conjugated Imidazole Compounds. *Chemistry Letters*, **2017**, 46, 1372-1375	1.7	6
163	Low-lying □ resonances associated with cyano groups: A CAP/SAC-CI study. *Chemical Physics*, **2017**, 482, 169-177	2.3	9

162	Intramolecular Hydroamination by a Primary Amine of an Unactivated Alkene on Gold Nanoclusters: A DFT Study. *ChemCatChem*, **2017**, 9, 4450-4450	5.2	
161	Regioselectivity of Sc2C2@C3v(8)-C82: Role of the Sumanene-Type Hexagon in Diels-Alder Reaction. *Journal of Organic Chemistry*, **2016**, 81, 8169-74	4.2	11
160	Structure, Interaction, and Dynamics of Au/Pd Bimetallic Nanoalloys Dispersed in Aqueous Ethylpyrrolidone, a Monomeric Moiety of Polyvinylpyrrolidone. *Journal of Physical Chemistry C*, **2016**, 120, 17454-17464	3.8	24
159	Multistep Intersystem Crossing Pathways in Cinnamate-Based UV-B Sunscreens. *Journal of Physical Chemistry Letters*, **2016**, 7, 4001-4007	6.4	27
158	Low-Lying Resonances of Standard and Rare DNA and RNA Bases Studied by the Projected CAP/SAC-CI Method. *Journal of Physical Chemistry A*, **2016**, 120, 1545-53	2.8	27
157	Coumarin-based donor cceptor organic dyes for a dye-sensitized solar cell: photophysical properties and electron injection mechanism. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	19
156	Warning to Theoretical Structure Elucidation of Endohedral Metallofullerenes. *Journal of Physical Chemistry C*, **2016**, 120, 1275-1283	3.8	25
155	Projected CAP/SAC-CI method with smooth Voronoi potential for calculating resonance states. *Journal of Computational Chemistry*, **2016**, 37, 242-9	3.5	15
154	Electronic Transitions in Conformationally Controlled Peralkylated Hexasilanes. *ChemPhysChem*, **2016**, 17, 3010-3022	3.2	14
153	Ability of density functional theory methods to accurately model the reaction energy pathways of the oxidation of CO on gold cluster: A benchmark study. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	11
152	Mechanism of Ullmann Coupling Reaction of Chloroarene on Au/Pd Alloy Nanocluster: A DFT Study. *Organometallics*, **2016**, 35, 1192-1201	3.8	15
151	Electronic excitation and ionization behavior of N-hydroxypyridine-2(1H)-thione and its deprotonated anion in a polarizable medium studied using quantum chemical computations. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	3
150	Sc3N@Cs(39715)-C82: a missing isomer linked to Sc3N@C2v(39718)-C82 by a single step Stone-Wales transformation. *RSC Advances*, **2016**, 6, 75588-75593	3.7	4
149	Modeling Molecular Systems at Extreme Pressure by an Extension of the Polarizable Continuum Model (PCM) Based on the Symmetry-Adapted Cluster-Configuration Interaction (SAC-CI) Method: Confined Electronic Excited States of Furan as a Test Case. *Journal of Chemical Theory and*	6.4	26
148	Synthesis and Optical Properties of Imidazole- and Benzimidazole-Based Fused -Conjugated Compounds: Influence of Substituent, Counteranion, and -Conjugated System. *Journal of Organic Chemistry*, **2015**, 80, 7172-83	4.2	18
147	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, 8593-602	16.4	22
146	Exploring excited states using Time Dependent Density Functional Theory and density-based indexes. *Coordination Chemistry Reviews*, **2015**, 304-305, 166-178	23.2	94
145	(2 + 2) Cycloaddition of Benzyne to Endohedral Metallofullerenes M3N@C80 (M = Sc, Y): A Rotating-Intermediate Mechanism. *Journal of the American Chemical Society*, **2015**, 137, 6820-8	16.4	33

144	Methane activation on Fe- and FeO-embedded graphene and boron nitride sheet: role of atomic defects in catalytic activities. *RSC Advances*, **2015**, 5, 97918-97927	3.7	21
143	Short-range stabilizing potential for computing energies and lifetimes of temporary anions with extrapolation methods. *Journal of Chemical Physics*, **2015**, 142, 034105	3.9	19
142	Nucleobases tagged to gold nanoclusters cause a mechanistic crossover in the oxidation of CO. *Physical Chemistry Chemical Physics*, **2015**, 17, 24275-81	3.6	7
141	Complex absorbing potentials with Voronoi isosurfaces wrapping perfectly around molecules. *Journal of Chemical Theory and Computation*, **2015**, 11, 4627-33	6.4	27
140	Proton-induced generation of remote N-heterocyclic carbene-Ru complexes. *Chemistry - A European Journal*, **2015**, 21, 106-10	4.8	8
139	Electronic excitation of molecules in solution calculated using the symmetry-adapted cluster□configuration interaction method in the polarizable continuum model **2015**,		3
138	Gold/Palladium Alloy for Carbon-Halogen Bond Activation: An Unprecedented Halide Dependence. *Chemistry - an Asian Journal*, **2015**, 10, 2669-76	4.5	10
137	Mechanism of the Aerobic Homocoupling of Phenylboronic Acid on Au□: A DFT Study. *Chemistry - an Asian Journal*, **2015**, 10, 2397-403	4.5	21
136	Gold/Palladium Bimetallic Nanoclusters for C-X Bond Activation: A Unique Effect of Gold. *Yuki Gosei Kagaku Kyokaishi/Journal of Synthetic Organic Chemistry*, **2015**, 73, 1130-1140	0.2	5
135	Electronic Structure and Transition in the Far-Ultraviolet Region **2015**, 29-54		1
134	Metal-porphyrin: a potential catalyst for direct decomposition of N(2)O by theoretical reaction mechanism investigation. *Environmental Science & Technology*, **2014**, 48, 7101-10	10.3	33
133	An efficient computational scheme for electronic excitation spectra of molecules in solution using the symmetry-adapted cluster-configuration interaction method: the accuracy of excitation energies and intuitive charge-transfer indices. *Journal of Chemical Physics*, **2014**, 141, 154104	3.9	10
132	Electronic transitions in conformationally controlled tetrasilanes with a wide range of SiSiSiSi dihedral angles. *Chemistry - A European Journal*, **2014**, 20, 9431-41	4.8	12
131	C□□l Bond Activation on Au/Pd Bimetallic Nanocatalysts Studied by Density Functional Theory and Genetic Algorithm Calculations. *Journal of Physical Chemistry C*, **2014**, 118, 22188-22196	3.8	38
130	Rydberg and □* transitions in film surfaces of various kinds of nylons studied by attenuated total reflection far-ultraviolet spectroscopy and quantum chemical calculations: peak shifts in the spectra and their relation to nylon structure and hydrogen bondings. *Journal of Physical Chemistry B*, **2014**, 118, 11855-61	3.4	28
129	Photophysical properties and photochemistry of substituted cinnamates and cinnamic acids for UVB blocking: effect of hydroxy, nitro, and fluoro substitutions at ortho, meta, and para positions. *Photochemical and Photobiological Sciences*, **2014**, 13, 583-94	4.2	22
128	Halogen exchange by reaction of CpRu(Cl)(PPh3)2 with MeC(O)X (X□=□Br, I) and its mechanistic study. *Journal of Organometallic Chemistry*, **2014**, 769, 34-37	2.3	6
127	Direct oxidation of methane to methanol on Fe□O modified graphene. *RSC Advances*, **2014**, 4, 12572-12578	3.7	40

126	Cooperative H2 Activation at Ag Cluster/Al2O3(110) Dual Perimeter Sites: A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2014**, 118, 7996-8006	3.8	28
125	Benchmark Study on the Triplet Excited-State Geometries and Phosphorescence Energies of Heterocyclic Compounds: Comparison Between TD-PBE0 and SAC-CI. *Journal of Chemical Theory and Computation*, **2014**, 10, 3969-79	6.4	32
124	Sumanenetrione Anions Generated by Electrochemical and Chemical Reduction. *Chemistry Letters*, **2014**, 43, 1297-1299	1.7	5
123	Electronic excitation spectra of molecules in solution calculated using the symmetry-adapted cluster-configuration interaction method in the polarizable continuum model with perturbative approach. *Journal of Chemical Physics*, **2014**, 140, 064114	3.9	10
122	Iodine molecule for neutrino mass spectroscopy: ab initio calculation of spectral rate. *Progress of Theoretical and Experimental Physics*, **2014**, 2014, 13B02-0	5.4	1
121	Communication: Coupled-cluster interpretation of the photoelectron spectrum of Au. *Journal of Chemical Physics*, **2014**, 141, 101102	3.9	6
120	Efficiency of perturbation-selection and its orbital dependence in the SAC-CI calculations for valence excitations of medium-size molecules. *Journal of Computational Chemistry*, **2014**, 35, 2163-76	3.5	20
119	Experimental and theoretical study on the excited-state dynamics of ortho-, meta-, and para-methoxy methylcinnamate. *Journal of Chemical Physics*, **2014**, 141, 244313	3.9	32
118	Mechanism of the aerobic oxidation of methanol to formic acid on Au8A DFT study. *International Journal of Quantum Chemistry*, **2013**, 113, 428-436	2.1	17
117	Linear response function approach for the boundary problem of QM/MM methods. *International Journal of Quantum Chemistry*, **2013**, 113, 336-341	2.1	4
116	Absorption and emission properties of various substituted cinnamic acids and cinnamates, based on TDDFT investigation. *International Journal of Quantum Chemistry*, **2013**, 113, 542-554	2.1	18
115	Chemically intuitive indices for charge-transfer excitation based on SAC-CI and TD-DFT calculations. *Journal of Computational Chemistry*, **2013**, 34, 2498-501	3.5	24
114	Aerobic oxidation of methanol to formic acid on Au8-: benchmark analysis based on completely renormalized coupled-cluster and density functional theory calculations. *Journal of Physical Chemistry A*, **2013**, 117, 10416-27	2.8	17
113	Electronic excited states and electronic spectra of biphenyl: a study using many-body wavefunction methods and density functional theories. *Physical Chemistry Chemical Physics*, **2013**, 15, 17426-34	3.6	19
112	Mechanisms for Solvatochromic Shifts of Free-Base Porphine Studied with Polarizable Continuum Models and Explicit Solute-Solvent Interactions. *Journal of Chemical Theory and Computation*, **2013**, 9, 470-80	6.4	16
111	Excited-State Geometries of Heteroaromatic Compounds: A Comparative TD-DFT and SAC-CI Study. *Journal of Chemical Theory and Computation*, **2013**, 9, 2368-79	6.4	54
110	Bond Metathesis between MX and RC(O)X? (M = Pt, Pd; X, X? = Cl, Br, I): Facile Determination of the Relative Values of the Oxidative Additions of RC(O)X to an M(0) Complex, Evidence by Density Functional Theory Calculations, and Synthetic Applications. *Organometallics*, **2013**, 32, 2026-2032	3.8	8
109	Polarization and site dependence of interatomic relaxation effects in double core hole states. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2013**, 46, 164012	1.3	4

108	Theoretical study of the electronic excitations of free-base porphyrin-Ar2 van der Waals complexes. *Journal of Chemical Physics*, **2013**, 139, 074303	3.9	3
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