Masahiro Ehara

List of Publications by Citations

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	Variational calculations of fermion second-order reduced density matrices by semidefinite programming algorithm. *Journal of Chemical Physics*, **2001**, 114, 8282-8292	3.9	217
250	Double-core-hole spectroscopy for chemical analysis with an intense X-ray femtosecond laser. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 16912-5	11.5	147
249	D□A-Type Organic Dyes for Dye-Sensitized Solar Cells with a Potential for Direct Electron Injection and a High Extinction Coefficient: Synthesis, Characterization, and Theoretical Investigation. *Journal of Physical Chemistry C*, **2012**, 116, 25653-25663	3.8	128
248	Low-temperature carbon-chlorine bond activation by bimetallic gold/palladium alloy nanoclusters: an application to Ullmann coupling. *Journal of the American Chemical Society*, **2012**, 134, 20250-3	16.4	119
247	Molecular double core hole electron spectroscopy for chemical analysis. *Journal of Chemical Physics* , **2010**, 132, 184302	3.9	103
246	Vibrationally resolved O 1s photoelectron spectrum of water. *Chemical Physics Letters*, **2003**, 380, 647-653	2.5	102
245	Double core hole creation and subsequent Auger decay in NH3 and CH4 molecules. *Physical Review Letters*, **2010**, 105, 213005	7.4	96
244	Exploring excited states using Time Dependent Density Functional Theory and density-based indexes. *Coordination Chemistry Reviews*, **2015**, 304-305, 166-178	23.2	94
243	Electronic excitation spectra of furan and pyrrole: Revisited by the symmetry adapted cluster□configuration interaction method. *Journal of Chemical Physics*, **2000**, 113, 7853-7866	3.9	82
242	Electronic excitations of the green fluorescent protein chromophore in its protonation states: SAC/SAC-CI study. *Journal of Computational Chemistry*, **2003**, 24, 1421-31	3.5	78
241	Density matrix variational theory: Application to the potential energy surfaces and strongly correlated systems. *Journal of Chemical Physics*, **2002**, 116, 5432-5439	3.9	78
240	Symmetry-adapted cluster and symmetry-adapted cluster-configuration interaction method in the polarizable continuum model: theory of the solvent effect on the electronic excitation of molecules in solution. *Journal of Chemical Physics*, **2010**, 133, 024104	3.9	70
239	Light-driven molecular switch for reconfigurable spin filters. *Nature Communications*, **2019**, 10, 2455	17.4	68
238	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
237	Outer- and inner-valence ionization spectra of N2 and CO:. *Chemical Physics Letters*, **1998**, 282, 347-354	2.5	60
236	Excited and Ionized States of p-Benzoquinone and Its Anion Radical: SAC□CI Theoretical Study. *Journal of Physical Chemistry A*, **2002**, 106, 3838-3849	2.8	55
235	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

234	Cluster modeling of metal oxides: how to cut out a cluster?. *Chemical Physics Letters*, **1998**, 291, 445-452	2.5	54
233	Multiconfiguration time-dependent Hartree (MCTDH) study on rotational and diffractive inelastic molecule-surface scattering. *Journal of Chemical Physics*, **1996**, 105, 8865-8877	3.9	54
232	Symmetry-dependent vibrational excitation in N 1s photoionization of N2: experiment and theory. *Journal of Chemical Physics*, **2006**, 124, 124311	3.9	52
231	Nonequilibrium solvation for vertical photoemission and photoabsorption processes using the symmetry-adapted cluster-configuration interaction method in the polarizable continuum model. *Journal of Chemical Physics*, **2011**, 134, 104109	3.9	50
230	Electronic excitation spectrum of thiophene studied by symmetry-adapted cluster configuration interaction method. *Journal of Chemical Physics*, **2001**, 114, 842	3.9	49
229	CAP/SAC-CI method for calculating resonance states of metastable anions. *Chemical Physics Letters*, **2012**, 537, 107-112	2.5	47
228	A Mechanism for the Palladium-Catalyzed Regioselective Silaboration of Allene: A Theoretical Study. *Organometallics*, **2008**, 27, 1736-1742	3.8	47
227	Singly and doubly excited states of butadiene, acrolein, and glyoxal: Geometries and electronic spectra. *Journal of Chemical Physics*, **2006**, 125, 014316	3.9	47
226	Theoretical fine spectroscopy with symmetry adapted cluster-configuration interaction general-R method: first-row K-shell ionizations and their satellites. *Journal of Chemical Physics*, **2005**, 122, 14304	3.9	47
225	Excited and ionized states of aniline: Symmetry adapted cluster configuration interaction theoretical study. *Journal of Chemical Physics*, **2002**, 117, 2045-2052	3.9	46
224	Theoretical study on the excited and ionized states of titanium tetrachloride. *Journal of Chemical Physics*, **1992**, 97, 2561-2570	3.9	45
223	Active-space symmetry-adapted-cluster configuration-interaction and equation-of-motion coupled-cluster methods for high accuracy calculations of potential energy surfaces of radicals. *Journal of Chemical Physics*, **2007**, 126, 164111	3.9	44
222	Electronic excitation and ionization spectra of azabenzenes: Pyridine revisited by the symmetry-adapted cluster configuration interaction method. *Journal of Chemical Physics*, **2001**, 114, 5117-5123	3.9	44
221	Theoretical fine spectroscopy with symmetry-adapted-cluster configuration-interaction method: outer- and inner-valence ionization spectra of furan, pyrrole, and thiophene. *Journal of Chemical Physics*, **2005**, 122, 234319	3.9	43
220	Theoretical study on the outer- and inner-valence ionization spectra of H2O, H2S and H2Se using the SAC-CI general-R method. *Journal of Chemical Physics*, **2001**, 114, 8990-8999	3.9	43
219	Symmetry-adapted cluster□configuration interaction method applied to high-spin multiplicity. *Journal of Chemical Physics*, **1993**, 98, 7179-7184	3.9	43
218	Elucidating electronic transitions from □rbitals of liquid n- and branched alkanes by far-ultraviolet spectroscopy and quantum chemical calculations. *Journal of Physical Chemistry A*, **2012**, 116, 11957-64	2.8	41
217	Symmetry adapted cluster-configuration interaction study on the excited and ionized states of TiBr4 and TiI4. *Journal of Chemical Physics*, **1994**, 101, 7658-7671	3.9	41

216	Direct oxidation of methane to methanol on Fe□ modified graphene. *RSC Advances*, **2014**, 4, 12572-12578	3.7	40
215	Double core□hole electron spectroscopy for open-shell molecules: Theoretical perspective. *Chemical Physics Letters*, **2010**, 496, 217-222	2.5	40
214	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
213	Vibrationally resolved C and O 1s photoelectron spectra of carbon dioxide. *Journal of Electron Spectroscopy and Related Phenomena*, **2007**, 155, 54-57	1.7	38
212	Aerobic oxidation of methanol to formic acid on Au20-: a theoretical study on the reaction mechanism. *Physical Chemistry Chemical Physics*, **2012**, 14, 3103-11	3.6	37
211	Iterative Cl general singles and doubles (ICIGSD) method for calculating the exact wave functions of the ground and excited states of molecules. *Journal of Chemical Physics*, **2005**, 122, 194108	3.9	37
210	Analytical energy gradients of the excited, ionized and electron-attached states calculated by the SAC-CI general-R method. *Chemical Physics Letters*, **2001**, 347, 493-498	2.5	36
209	Structure of the exact wave function. V. Iterative configuration interaction method for molecular systems within finite basis. *Journal of Chemical Physics*, **2002**, 117, 9-12	3.9	36
208	Photoisomerization and proton-coupled electron transfer (PCET) promoted water oxidation by mononuclear cyclometalated ruthenium catalysts. *Inorganic Chemistry*, **2012**, 51, 5386-92	5.1	34
207	Analytical energy gradient of the symmetry-adapted-cluster configuration-interaction general-R method for singlet to septet ground and excited states. *Journal of Chemical Physics*, **2004**, 120, 2593-605	3.9	34
206	(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
205	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
204	Electronic transitions in liquid amides studied by using attenuated total reflection far-ultraviolet spectroscopy and quantum chemical calculations. *Journal of Chemical Physics*, **2013**, 139, 154301	3.9	33
203	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
202	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
201	Peralkylated Tetrasilanes:□Conformational Dependence of the Photoelectron Spectrum□ *Journal of Physical Chemistry A*, **2002**, 106, 2369-2373	2.8	32
200	Electronic excitation and ionization spectra of cyclopentadiene: Revisit by the symmetry-adapted cluster□onfiguration interaction method. *Journal of Chemical Physics*, **2000**, 113, 5245	3.9	32
199	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

198	Excited states and electronic spectra of extended tetraazaporphyrins. *Journal of Chemical Physics*, **2010**, 133, 144316	3.9	31
197	Singularity-free analytical energy gradients for the SAC/SAC-CI method: coupled perturbed minimum orbital-deformation (CPMOD) approach. *Chemical Physics Letters*, **2003**, 367, 730-736	2.5	31
196	Fine theoretical spectroscopy using symmetry adapted cluster-configuration interaction general-R method: Outer- and inner-valence ionization spectra of CS2 and OCS. *Journal of Chemical Physics*, **2002**, 117, 3248-3255	3.9	31
195	SAC-CI GENERAL-R METHOD: THEORY AND APPLICATIONS TO THE MULTI-ELECTRON PROCESSES **2002**, 293-319		31
194	Direct determination of second-order density matrix using density equation: Open-shell system and excited state. *Journal of Chemical Physics*, **2000**, 112, 8772-8778	3.9	31
193	SAC□I theoretical investigation on electronic structure of fluorene□hiophene oligomers. *Polymer*, **2005**, 46, 6474-6481	3.9	30
192	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
191	Theoretical molecular double-core-hole spectroscopy of nucleobases. *Journal of Physical Chemistry A*, **2011**, 115, 12070-82	2.8	29
190	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
189	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
188	Complex absorbing potentials with Voronoi isosurfaces wrapping perfectly around molecules. *Journal of Chemical Theory and Computation*, **2015**, 11, 4627-33	6.4	27
187	Multistep Intersystem Crossing Pathways in Cinnamate-Based UV-B Sunscreens. *Journal of Physical Chemistry Letters*, **2016**, 7, 4001-4007	6.4	27
186	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
185	Theoretical spectroscopy on K□, K□L□, and L□ double core hole states of SiX4 (X=H, F, Cl, and CH3) molecules. *Chemical Physics*, **2011**, 384, 28-35	2.3	27
184	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 Computation*, **2015**, 11, 2063-76	6.4	26
183	Double core□ole correlation satellite spectra of N2 and CO molecules. *Chemical Physics Letters*, **2012**, 521, 45-51	2.5	26
182	Warning to Theoretical Structure Elucidation of Endohedral Metallofullerenes. *Journal of Physical Chemistry C*, **2016**, 120, 1275-1283	3.8	25
181	Absorption and emission spectra of ultraviolet B blocking methoxy substituted cinnamates investigated using the symmetry-adapted cluster configuration interaction method. *Journal of Chemical Physics*, **2009**, 131, 224306	3.9	25

180	Hyperfine splitting constants studied by the symmetry adapted cluster-configuration interaction method. *Journal of Chemical Physics*, **1994**, 100, 5821-5828	3.9	25
179	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
178	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
177	Auger decay of molecular double core-hole state. *Journal of Chemical Physics*, **2011**, 135, 154307	3.9	24
176	Investigation of the electronic spectra and excited-state geometries of poly(para-phenylene vinylene) (PPV) and poly(para-phenylene) (PP) by the symmetry-adapted cluster configuration interaction (SAC-CI) method. *Journal of Physical Chemistry A*, **2007**, 111, 5473-81	2.8	24
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174	Possible reaction pathway in methanol dehydrogenation on Pt and Ag surfaces/clusters starting from OH scission: Dipped adcluster model study. *Surface Science*, **2009**, 603, 641-646	1.8	23
173	Elimination of singularities in molecular orbital derivatives: minimum orbital-deformation (MOD) method. *Chemical Physics Letters*, **2002**, 356, 1-6	2.5	23
172	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
171	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
170	Catalysis of Cu Cluster for NO Reduction by CO: Theoretical Insight into the Reaction Mechanism. *ACS Omega*, **2019**, 4, 2596-2609	3.9	21
169	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
168	Mechanism of the Aerobic Homocoupling of Phenylboronic Acid on Au A DFT Study. *Chemistry - an Asian Journal*, **2015**, 10, 2397-403	4.5	21
167	Enhancement of catalytic reactivity of zinc(II) complex by a cyclotriveratrylene-capped structure. *Journal of Organometallic Chemistry*, **2012**, 706-707, 26-29	2.3	21
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165	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
164	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
163	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

162	Nonradiative decay dynamics of methyl-4-hydroxycinnamate and its hydrated complex revealed by picosecond pump-probe spectroscopy. *Physical Chemistry Chemical Physics*, **2012**, 14, 8999-9005	3.6	20
161	Ionization spectrum of CO2 studied by the SAC-CI general-R method. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **1999**, 55, 487-493	4.4	20
160	Theoretical study on 31P NMR chemical shifts of phosphorus-modified CHA zeolites. *Microporous and Mesoporous Materials*, **2020**, 294, 109908	5.3	20
159	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
158	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
157	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
156	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
155	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
154	Ab initio study of the excited singlet states of all-trans alpha,omega-diphenylpolyenes with one to seven polyene double bonds: Simulation of the spectral data within Franck-Condon approximation. *Journal of Chemical Physics*, **2009**, 131, 174313	3.9	19
153	Auger decay of molecular double core-hole and its satellite states: comparison of experiment and calculation. *Journal of Chemical Physics*, **2012**, 137, 224306	3.9	19
152	Outer- and inner-valence ionization spectra of NH3, PH3, and AsH3: symmetry-adapted cluster configuration interaction general-R study. *Journal of Chemical Physics*, **2002**, 116, 1934-1943	3.9	19
151	New aspects of the photodissociation of water in the first absorption band: How strong is excitation of the first triplet state?. *Journal of Chemical Physics*, **1998**, 109, 6641-6646	3.9	19
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149	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
148	Enantioseparation and chiral induction in Ag nanoclusters with intrinsic chirality. *Chemical Science*, **2020**, 11, 2394-2400	9.4	18
147	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
146	Theoretical Insights into Monometallofullerene Th@C: Strong Covalent Interaction between Thorium and the Carbon Cage. *Inorganic Chemistry*, **2018**, 57, 2961-2964	5.1	17
145	Mechanism of the aerobic oxidation of methanol to formic acid on Au8□A DFT study. *International Journal of Quantum Chemistry*, **2013**, 113, 428-436	2.1	17

144	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
143	Collision induced absorption spectra and line broadening of CsRg system (Rg=Xe, Kr, Ar, Ne) studied by the symmetry adapted cluster-configuration interaction (SAC-Cl) method. *Journal of Chemical Physics*, **1995**, 102, 6822-6830	3.9	17
142	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
141	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
140	ESIPT emission behavior of methoxy-substituted 2-hydroxyphenylbenzimidazole isomers. *New Journal of Chemistry*, **2018**, 42, 5923-5928	3.6	16
139	Different photoisomerization routes found in the structural isomers of hydroxy methylcinnamate. *Physical Chemistry Chemical Physics*, **2018**, 20, 17583-17598	3.6	16
138	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
137	Ground and excited states of singlet, cation doublet, and anion doublet states of o-benzoquinone: a theoretical study. *Journal of Physical Chemistry A*, **2007**, 111, 2634-9	2.8	16
136	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
135	Optical absorption and fluorescence of PRODAN in solution: Quantum chemical study based on the symmetry-adapted cluster-configuration interaction method. *Chemical Physics Letters*, **2012**, 552, 53-57	2.5	15
134	Low-lying valence excited states of CNC, C2N, N3, and NCO studied using the electron-attached and ionized symmetry-adapted-cluster configuration-interaction and equation-of-motion coupled-cluster methodologies. *Molecular Physics*, **2009**, 107, 871-880	1.7	15
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131	CASSCF study of bonding in NiCO and FeCO. *International Journal of Quantum Chemistry*, **1999**, 72, 221-231	2.1	15
130	Projected CAP/SAC-CI method with smooth Voronoi potential for calculating resonance states. *Journal of Computational Chemistry*, **2016**, 37, 242-9	3.5	15
129	Mechanism of Ullmann Coupling Reaction of Chloroarene on Au/Pd Alloy Nanocluster: A DFT Study. *Organometallics*, **2016**, 35, 1192-1201	3.8	15
128	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
127	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

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124	Ni-Catalyzed Dimerization and Hydroperfluoroarylation of 1,3-Dienes. *Journal of Organic Chemistry*, **2018**, 83, 9267-9277	4.2	13
123	Comparative study of C^N and N^C type cyclometalated ruthenium complexes with a NAD+/NADH function. *Inorganic Chemistry*, **2012**, 51, 8091-102	5.1	13
122	Electronic excitations of C60 fullerene calculated using the ab initio cluster expansion method. *Journal of Chemical Physics*, **2012**, 137, 134304	3.9	13
121	Diels-Alder Cycloaddition of Cyclopentadiene and C at the Extreme High Pressure. *Journal of Physical Chemistry A*, **2017**, 121, 4363-4371	2.8	12
120	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
119	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
118	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
117	Interatomic relaxation effects in double core ionization of chain molecules. *Journal of Chemical Physics*, **2012**, 137, 154316	3.9	12
116	Electronic transitions in cis- and trans-dichloroethylenes and tetrachloroethylene. *Journal of Chemical Physics*, **2008**, 129, 174506	3.9	12
115	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
114	Crystallographic Characterization of ErC@C: Cluster Stretching with Cage Elongation. *Inorganic Chemistry*, **2020**, 59, 1940-1946	5.1	11
113	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
112	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
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110	Valence ionized states of iron pentacarbonyl and eta5-cyclopentadienyl cobalt dicarbonyl studied by symmetry-adapted cluster-configuration interaction calculation and collision-energy resolved Penning ionization electron spectroscopy. *Journal of Chemical Physics*, **2010**, 132, 084302	3.9	11
109	Relativistic effects in K-shell ionizations: SAC-CI general-R study based on the DK2 Hamiltonian. *Chemical Physics*, **2009**, 356, 195-198	2.3	11

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107	Electronic spectra and photodissociation of vinyl chloride: a symmetry-adapted cluster configuration interaction study. *Journal of Chemical Physics*, **2006**, 124, 034312	3.9	11
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