# Masahiro Ehara

List of Publications by Year
in descending order

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| 264 | 6,432 | 71061 | 123376 |
|---|---|---|---|
| papers | citations | 41 h-index | 61 g-index |

| 278 | 278 | 278 | 5717 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Variational calculations of fermion second-order reduced density matrices by semidefinite programming algorithm. Journal of Chemical Physics, 2001, 114, 8282-8292. | 1.2 | 239 |
| 2 | 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, 16912-16915. | 3.3 | 165 |
| 3 | Dâ€“Dâˆ’Îâ€“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. | 1.5 | 153 |
| 4 | Low-Temperature Carbonâ€“Chlorine Bond Activation by Bimetallic Gold/Palladium Alloy Nanoclusters: An Application to Ullmann Coupling. Journal of the American Chemical Society, 2012, 134, 20250-20253. | 6.6 | 133 |
| 5 | Vibrationally resolved O 1s photoelectron spectrum of water. Chemical Physics Letters, 2003, 380, 647-653. | 1.2 | 119 |
| 6 | Exploring excited states using Time Dependent Density Functional Theory and density-based indexes. Coordination Chemistry Reviews, 2015, 304-305, 166-178. | 9.5 | 118 |
| 7 | Molecular double core hole electron spectroscopy for chemical analysis. Journal of Chemical Physics, 2010, 132, . | 1.2 | 111 |
| 8 | Light-driven molecular switch for reconfigurable spin filters. Nature Communications, 2019, 10, 2455. | 5.8 | 109 |
| 9 | Double Core Hole Creation and Subsequent Auger Decay in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>NH</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CH</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math>Molecules. Physical Review Letters, 2010, 105, 213005. | 2.9 | 105 |
| 10 | Electronic excitation spectra of furan and pyrrole: Revisited by the symmetry adapted clusterâ€“configuration interaction method. Journal of Chemical Physics, 2000, 113, 7853-7866. | 1.2 | 88 |
| 11 | Electronic excitations of the green fluorescent protein chromophore in its protonation states: SAC/SAC-CI study. Journal of Computational Chemistry, 2003, 24, 1421-1431. | 1.5 | 83 |
| 12 | Density matrix variational theory: Application to the potential energy surfaces and strongly correlated systems. Journal of Chemical Physics, 2002, 116, 5432-5439. | 1.2 | 79 |
| 13 | A Theoretical Investigation on CO Oxidation by Singleâ€Atom Catalysts M<sub>1</sub>/Î³â€Al<sub>2</sub>O<sub>3</sub> (M=Pd, Fe, Co, and Ni). ChemCatChem, 2017, 9, 1222-1229. | 1.8 | 76 |
| 14 | 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. | 1.2 | 71 |
| 15 | Outer- and inner-valence ionization spectra of N2 and CO:. Chemical Physics Letters, 1998, 282, 347-354. | 1.2 | 65 |
| 16 | Multiconfiguration timeâ€dependent Hartree (MCTDH) study on rotational and diffractive inelastic moleculeâ€surface scattering. Journal of Chemical Physics, 1996, 105, 8865-8877. | 1.2 | 61 |
| 17 | Excited and Ionized States of p-Benzoquinone and Its Anion Radical:â€‰ SACâˆ’CI Theoretical Study. Journal of Physical Chemistry A, 2002, 106, 3838-3849. | 1.1 | 61 |
| 18 | CAP/SAC-CI method for calculating resonance states of metastable anions. Chemical Physics Letters, 2012, 537, 107-112. | 1.2 | 59 |

| # | Article | IF | Citations |
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| 19 | Symmetry-dependent vibrational excitation in N 1s photoionization of N2: Experiment and theory. Journal of Chemical Physics, 2006, 124, 124311. | 1.2 | 57 |
| 20 | Excited-State Geometries of Heteroaromatic Compounds: A Comparative TD-DFT and SAC-CI Study. Journal of Chemical Theory and Computation, 2013, 9, 2368-2379. | 2.3 | 57 |
| 21 | Cluster modeling of metal oxides: how to cut out a cluster?. Chemical Physics Letters, 1998, 291, 445-452. | 1.2 | 54 |
| 22 | Singly and doubly excited states of butadiene, acrolein, and glyoxal: Geometries and electronic spectra. Journal of Chemical Physics, 2006, 125, 014316. | 1.2 | 54 |
| 23 | Lewis Acid Catalysis of Nb<sub>2</sub>O<sub>5</sub> for Reactions of Carboxylic Acid Derivatives in the Presence of Basic Inhibitors. ChemCatChem, 2019, 11, 383-396. | 1.8 | 53 |
| 24 | Excited and ionized states of aniline: Symmetry adapted cluster configuration interaction theoretical study. Journal of Chemical Physics, 2002, 117, 2045-2052. | 1.2 | 52 |
| 25 | Nonequilibrium solvation for vertical photoemission and photoabsorption processes using the symmetry-adapted clusterâ€“configuration interaction method in the polarizable continuum model. Journal of Chemical Physics, 2011, 134, 104109. | 1.2 | 51 |
| 26 | Elucidating Electronic Transitions from Ïƒ Orbitals of Liquid n- and Branched Alkanes by Far-Ultraviolet Spectroscopy and Quantum Chemical Calculations. Journal of Physical Chemistry A, 2012, 116, 11957-11964. | 1.1 | 51 |
| 27 | Theoretical fine spectroscopy with symmetry adapted clusterâ€“configuration interaction general-R method: First-row K-shell ionizations and their satellites. Journal of Chemical Physics, 2005, 122, 014304. | 1.2 | 50 |
| 28 | Direct oxidation of methane to methanol on Feâ€“O modified graphene. RSC Advances, 2014, 4, 12572-12578. | 1.7 | 50 |
| 29 | Electronic excitation spectrum of thiophene studied by symmetry-adapted cluster configuration interaction method. Journal of Chemical Physics, 2001, 114, 842. | 1.2 | 49 |
| 30 | Theoretical study on the excited and ionized states of titanium tetrachloride. Journal of Chemical Physics, 1992, 97, 2561-2570. | 1.2 | 47 |
| 31 | 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. | 1.2 | 47 |
| 32 | A Mechanism for the Palladium-Catalyzed Regioselective Silaboration of Allene: A Theoretical Study. Organometallics, 2008, 27, 1736-1742. | 1.1 | 47 |
| 33 | 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. | 1.2 | 46 |
| 34 | 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. | 1.2 | 45 |
| 35 | 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. | 3.7 | 45 |
| 36 | Symmetry adapted clusterâ€configuration interaction study on the excited and ionized states of TiBr4 and TiI4. Journal of Chemical Physics, 1994, 101, 7658-7671. | 1.2 | 44 |

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| 37 | 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. | 1.2 | 44 |
| 38 | Double coreâ€“hole electron spectroscopy for open-shell molecules: Theoretical perspective. Chemical Physics Letters, 2010, 496, 217-222. | 1.2 | 44 |
| 39 | Metalâ€“Porphyrin: A Potential Catalyst for Direct Decomposition of N<sub>2</sub>O by Theoretical Reaction Mechanism Investigation. Environmental Science & Technology, 2014, 48, 7101-7110. | 4.6 | 44 |
| 40 | Symmetryâ€adapted clusterâ€“configuration interaction method applied to highâ€spin multiplicity. Journal of Chemical Physics, 1993, 98, 7179-7184. | 1.2 | 43 |
| 41 | Complex Absorbing Potentials with Voronoi Isosurfaces Wrapping Perfectly around Molecules. Journal of Chemical Theory and Computation, 2015, 11, 4627-4633. | 2.3 | 43 |
| 42 | Vibrationally resolved C and O 1s photoelectron spectra of carbon dioxide. Journal of Electron Spectroscopy and Related Phenomena, 2007, 155, 54-57. | 0.8 | 41 |
| 43 | 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. | 1.2 | 41 |
| 44 | Aerobic oxidation of methanol to formic acid on Au20â^': a theoretical study on the reaction mechanism. Physical Chemistry Chemical Physics, 2012, 14, 3103. | 1.3 | 40 |
| 45 | Câ€“Cl 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. | 1.5 | 39 |
| 46 | Photoisomerization and Proton-Coupled Electron Transfer (PCET) Promoted Water Oxidation by Mononuclear Cyclometalated Ruthenium Catalysts. Inorganic Chemistry, 2012, 51, 5386-5392. | 1.9 | 38 |
| 47 | (2 + 2) Cycloaddition of Benzyne to Endohedral Metallofullerenes M<sub>3</sub>N@C<sub>80</sub> (M = Sc, Y): A Rotating-Intermediate Mechanism. Journal of the American Chemical Society, 2015, 137, 6820-6828. | 6.6 | 38 |
| 48 | 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. | 1.7 | 38 |
| 49 | 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. | 1.2 | 37 |
| 50 | 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. | 1.2 | 37 |
| 51 | Iterative CI 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. | 1.2 | 37 |
| 52 | Excited states and electronic spectra of extended tetraazaporphyrins. Journal of Chemical Physics, 2010, 133, 144316. | 1.2 | 37 |
| 53 | Rydberg and Ï€â€“Ï€* 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, 11855-11861. | 1.2 | 37 |
| 54 | Enantioseparation and chiral induction in Ag<sub>29</sub> nanoclusters with intrinsic chirality. Chemical Science, 2020, 11, 2394-2400. | 3.7 | 37 |

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| 55 | Experimental and theoretical study on the excited-state dynamics of ortho-, meta-, and para-methoxy methylcinnamate. Journal of Chemical Physics, 2014, 141, 244313. | 1.2 | 36 |
| 56 | 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, 3969-3979. | 2.3 | 36 |
| 57 | Low-Lying Ï€* Resonances of Standard and Rare DNA and RNA Bases Studied by the Projected CAP/SACâ€“CI Method. Journal of Physical Chemistry A, 2016, 120, 1545-1553. | 1.1 | 36 |
| 58 | Catalysis of Cu Cluster for NO Reduction by CO: Theoretical Insight into the Reaction Mechanism. ACS Omega, 2019, 4, 2596-2609. | 1.6 | 36 |
| 59 | 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, 2593-2605. | 1.2 | 34 |
| 60 | Synthesis and Optical Properties of Excited-State Intramolecular Proton Transfer Active Ï€-Conjugated Benzimidazole Compounds: Influence of Structural Rigidification by Ring Fusion. Journal of Organic Chemistry, 2017, 82, 12173-12180. | 1.7 | 34 |
| 61 | Electronic excitation and ionization spectra of cyclopentadiene: Revisit by the symmetry-adapted clusterâ€“configuration interaction method. Journal of Chemical Physics, 2000, 113, 5245. | 1.2 | 33 |
| 62 | SAC-CI GENERAL-R METHOD: THEORY AND APPLICATIONS TO THE MULTI-ELECTRON PROCESSES. , 2002, , 293-319. | | 33 |
| 63 | Peralkylated Tetrasilanes:Â Conformational Dependence of the Photoelectron Spectrumâ€. Journal of Physical Chemistry A, 2002, 106, 2369-2373. | 1.1 | 33 |
| 64 | Multistep Intersystem Crossing Pathways in Cinnamate-Based UV-B Sunscreens. Journal of Physical Chemistry Letters, 2016, 7, 4001-4007. | 2.1 | 33 |
| 65 | Direct determination of second-order density matrix using density equation: Open-shell system and excited state. Journal of Chemical Physics, 2000, 112, 8772-8778. | 1.2 | 32 |
| 66 | 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. | 1.2 | 32 |
| 67 | 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. | 1.2 | 32 |
| 68 | SACâ€“CI theoretical investigation on electronic structure of fluoreneâ€“thiophene oligomers. Polymer, 2005, 46, 6474-6481. | 1.8 | 32 |
| 69 | Theoretical Molecular Double-Core-Hole Spectroscopy of Nucleobases. Journal of Physical Chemistry A, 2011, 115, 12070-12082. | 1.1 | 32 |
| 70 | Cooperative H<sub>2</sub> Activation at Ag Cluster/Î¸-Al<sub>2</sub>O<sub>3</sub>(110) Dual Perimeter Sites: A Density Functional Theory Study. Journal of Physical Chemistry C, 2014, 118, 7996-8006. | 1.5 | 31 |
| 71 | Modeling Molecular Systems at Extreme Pressure by an Extension of the Polarizable Continuum Model (PCM) Based on the Symmetry-Adapted Cluster-Configuration Interaction (SACâ€“CI) Method: Confined Electronic Excited States of Furan as a Test Case. Journal of Chemical Theory and Computation, 2015, 11, 2063-2076. | 2.3 | 31 |
| 72 | Potential molecular semiconductor devices: cyclo-C<sub>n</sub> (n = 10 and 14) with higher stabilities and aromaticities than acknowledged cyclo-C<sub>18</sub>. Physical Chemistry Chemical Physics, 2020, 22, 4823-4831. | 1.3 | 31 |

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| 73 | 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, 5473-5481. | 1.1 | 30 |
| 74 | Asymmetric Twisting of C-Centered Octahedral Gold(I) Clusters by Chiral N-Heterocyclic Carbene Ligation. Journal of the American Chemical Society, 2022, 144, 2156-2163. | 6.6 | 30 |
| 75 | Warning to Theoretical Structure Elucidation of Endohedral Metallofullerenes. Journal of Physical Chemistry C, 2016, 120, 1275-1283. | 1.5 | 29 |
| 76 | Preferential Photoreaction in a Porous Crystal, Metalâ€“Macrocycle Framework: Pd<sup>II</sup>-Mediated Olefin Migration over [2+2] Cycloaddition. Journal of the American Chemical Society, 2018, 140, 16610-16614. | 6.6 | 29 |
| 77 | Double coreâ€“hole correlation satellite spectra of N2 and CO molecules. Chemical Physics Letters, 2012, 521, 45-51. | 1.2 | 28 |
| 78 | 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, 583-594. | 1.6 | 28 |
| 79 | Short-range stabilizing potential for computing energies and lifetimes of temporary anions with extrapolation methods. Journal of Chemical Physics, 2015, 142, 034105. | 1.2 | 28 |
| 80 | Origin of Nb<sub>2</sub>O<sub>5</sub> Lewis Acid Catalysis for Activation of Carboxylic Acids in the Presence of a Hard Base. ChemPhysChem, 2018, 19, 2848-2857. | 1.0 | 28 |
| 81 | Theoretical spectroscopy on Kâ€“2, Kâ€“1Lâ€“1, and Lâ€“2 double core hole states of SiX4 (X=H, F, Cl, and CH3) molecules. Chemical Physics, 2011, 384, 28-35. | 0.9 | 27 |
| 82 | Chemically intuitive indices for charge-transfer excitation based on SAC-CI and TD-DFT calculations. Journal of Computational Chemistry, 2013, 34, 2498-2501. | 1.5 | 27 |
| 83 | Mechanism of the Aerobic Homocoupling of Phenylboronic Acid on Au<sub>20</sub><sup>â^</sup>: A DFT Study. Chemistry - an Asian Journal, 2015, 10, 2397-2403. | 1.7 | 27 |
| 84 | ESIPT emission behavior of methoxy-substituted 2-hydroxyphenylbenzimidazole isomers. New Journal of Chemistry, 2018, 42, 5923-5928. | 1.4 | 27 |
| 85 | Deep learning enabled inorganic material generator. Physical Chemistry Chemical Physics, 2020, 22, 26935-26943. | 1.3 | 27 |
| 86 | 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. | 1.2 | 26 |
| 87 | 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. | 1.5 | 26 |
| 88 | High Turnover Frequency COâ€“NO Reactions over Rh Overlayer Catalysts: A Comparative Study Using Rh Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 6080-6089. | 1.5 | 26 |
| 89 | Theoretical study on 31P NMR chemical shifts of phosphorus-modified CHA zeolites. Microporous and Mesoporous Materials, 2020, 294, 109908. | 2.2 | 26 |
| 90 | Crystallographic Characterization of Er<sub>2</sub>C<sub>2</sub>@C<sub>80â€“88</sub>: Cluster Stretching with Cage Elongation. Inorganic Chemistry, 2020, 59, 1940-1946. | 1.9 | 26 |

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| 91 | Hyperfine splitting constants studied by the symmetry adapted clusterâ€configuration interaction method. Journal of Chemical Physics, 1994, 100, 5821-5828. | 1.2 | 25 |
| 92 | Auger decay of molecular double core-hole state. Journal of Chemical Physics, 2011, 135, 154307. | 1.2 | 25 |
| 93 | Synthesis and Optical Properties of Imidazole- and Benzimidazole-Based Fused Ï€-Conjugated Compounds: Influence of Substituent, Counteranion, and Ï€-Conjugated System. Journal of Organic Chemistry, 2015, 80, 7172-7183. | 1.7 | 25 |
| 94 | How Can We Understand Au<sub>8</sub> Cores and Entangled Ligands of Selenolate- and Thiolate-Protected Gold Nanoclusters Au<sub>24</sub>(ER)<sub>20</sub> and Au<sub>20</sub>(ER)<sub>16</sub> (E = Se, S; R = Ph, Me)? A Theoretical Study. Journal of the American Chemical Society, 2015, 137, 8593-8602. | 6.6 | 25 |
| 95 | Changes in the Electronic States of Low-Temperature Solid n-Tetradecane: Decrease in the HOMOâ€“LUMO Gap. ACS Omega, 2017, 2, 618-625. | 1.6 | 25 |
| 96 | Nonradiative decay dynamics of methyl-4-hydroxycinnamate and its hydrated complex revealed by picosecond pumpâ€“probe spectroscopy. Physical Chemistry Chemical Physics, 2012, 14, 8999. | 1.3 | 24 |
| 97 | Silicon-coordinated nitrogen-doped graphene as a promising metal-free catalyst for N<sub>2</sub>O reduction by CO: a theoretical study. RSC Advances, 2018, 8, 22322-22330. | 1.7 | 24 |
| 98 | Reaction Behavior of the NO Molecule on the Surface of an M<sub>n</sub> Particle (M = Ru,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Journal of Physical Chemistry A, 2019, 123, 7021-7033. | 1.1 | 24 |
| 99 | Elimination of singularities in molecular orbital derivatives: minimum orbital-deformation (MOD) method. Chemical Physics Letters, 2002, 356, 1-6. | 1.2 | 23 |
| 100 | Possible reaction pathway in methanol dehydrogenation on Pt and Ag surfaces/clusters starting from Oâ€“H scission: Dipped adcluster model study. Surface Science, 2009, 603, 641-646. | 0.8 | 23 |
| 101 | Enhancement of catalytic reactivity of zinc(II) complex by a cyclotriveratrylene-capped structure. Journal of Organometallic Chemistry, 2012, 706-707, 26-29. | 0.8 | 23 |
| 102 | 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. | 1.3 | 23 |
| 103 | Coumarin-based donorâ€“Ï€â€“acceptor organic dyes for a dye-sensitized solar cell: photophysical properties and electron injection mechanism. Theoretical Chemistry Accounts, 2016, 135, 1. | 0.5 | 23 |
| 104 | Crystallographic characterization of Er<sub>2</sub>C<sub>2</sub>@C<sub>2</sub>(43)-C<sub>90</sub>, Er<sub>2</sub>C<sub>2</sub>@C<sub>2</sub>(40)-C<sub>90</sub>, Er<sub>2</sub>C<sub>2</sub>@C<sub>2</sub>(44)-C<sub>90</sub>, and Er<sub>2</sub>C<sub>2</sub>@C<sub>1</sub>(21)-C<sub>90</sub>: the role of cage-shape on cluster configuration. Nanoscale, 2019, 11, 17319-17326. | 2.8 | 23 |
| 105 | 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. | 1.2 | 22 |
| 106 | Theoretical Insights into Monometallofullerene Th@C<sub>76</sub>: Strong Covalent Interaction between Thorium and the Carbon Cage. Inorganic Chemistry, 2018, 57, 2961-2964. | 1.9 | 22 |
| 107 | Ni-Catalyzed Dimerization and Hydroperfluoroarylation of 1,3-Dienes. Journal of Organic Chemistry, 2018, 83, 9267-9277. | 1.7 | 22 |
| 108 | Enhanced oxygen reduction activity of platinum subnanocluster catalysts through charge redistribution. Chemical Communications, 2019, 55, 12603-12606. | 2.2 | 22 |

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| 109 | Ionization spectra of XONO2 (X=F, Cl, Br, I) studied by the SACâ€“CI method. Chemical Physics, 1998, 226, 113-123. | 0.9 | 21 |
| 110 | Ground and Excited States of Singlet, Cation Doublet, and Anion Doublet States ofo-Benzoquinone:Â A Theoretical Study. Journal of Physical Chemistry A, 2007, 111, 2634-2639. | 1.1 | 21 |
| 111 | Auger decay of molecular double core-hole and its satellite states: Comparison of experiment and calculation. Journal of Chemical Physics, 2012, 137, 224306. | 1.2 | 21 |
| 112 | Absorption and emission properties of various substituted cinnamic acids and cinnamates, based on TDDFT investigation. International Journal of Quantum Chemistry, 2013, 113, 542-554. | 1.0 | 21 |
| 113 | Ionization spectrum of CO2 studied by the SAC-CI general-R method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 487-493. | 2.0 | 20 |
| 114 | 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. | 1.2 | 20 |
| 115 | Ab initio study of the excited singlet states of all-trans Î±,Ï‰-diphenylpolyenes with one to seven polyene double bonds: Simulation of the spectral data within Franckâ€“Condon approximation. Journal of Chemical Physics, 2009, 131, 174313. | 1.2 | 20 |
| 116 | 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, 2163-2176. | 1.5 | 20 |
| 117 | Different photoisomerization routes found in the structural isomers of hydroxy methylcinnamate. Physical Chemistry Chemical Physics, 2018, 20, 17583-17598. | 1.3 | 20 |
| 118 | Influence of local strain caused by cycloaddition on the band gap control of functionalized single-walled carbon nanotubes. RSC Advances, 2019, 9, 13998-14003. | 1.7 | 20 |
| 119 | Collision induced absorption spectra and line broadening of CsRg system (Rg=Xe, Kr, Ar, Ne) studied by the symmetry adapted clusterâ€configuration interaction (SACâ€CI) method. Journal of Chemical Physics, 1995, 102, 6822-6830. | 1.2 | 19 |
| 120 | Projected <scp>CAP</scp>/<scp>SAC</scp>â€<scp>CI</scp> method with smooth <scp>V</scp>oronoi potential for calculating resonance states. Journal of Computational Chemistry, 2016, 37, 242-249. | 1.5 | 19 |
| 121 | Mechanism of the aerobic oxidation of methanol to formic acid on Au<sub>8</sub><sup>â^'</sup>: A DFT study. International Journal of Quantum Chemistry, 2013, 113, 428-436. | 1.0 | 18 |
| 122 | Aerobic Oxidation of Methanol to Formic Acid on Au<sub>8</sub><sup>â€“</sup>: Benchmark Analysis Based on Completely Renormalized Coupled-Cluster and Density Functional Theory Calculations. Journal of Physical Chemistry A, 2013, 117, 10416-10427. | 1.1 | 18 |
| 123 | Probing the electronic structures of Co<sub>n</sub> (n = 1â€“5) clusters on Î³-Al<sub>2</sub>O<sub>3</sub> surfaces using first-principles calculations. Physical Chemistry Chemical Physics, 2017, 19, 3679-3687. | 1.3 | 18 |
| 124 | Dielsâ€“Alder Cycloaddition of Cyclopentadiene and C<sub>60</sub> at the Extreme High Pressure. Journal of Physical Chemistry A, 2017, 121, 4363-4371. | 1.1 | 18 |
| 125 | The direct observation of the doorway <sup>1</sup>nÏ€* state of methylcinnamate and hydrogen-bonding effects on the photochemistry of cinnamate-based sunscreens. Physical Chemistry Chemical Physics, 2019, 21, 19755-19763. | 1.3 | 18 |
| 126 | Mechanisms for Solvatochromic Shifts of Free-Base Porphine Studied with Polarizable Continuum Models and Explicit Soluteâ€“Solvent Interactions. Journal of Chemical Theory and Computation, 2013, 9, 470-480. | 2.3 | 17 |

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| 127 | Analytical energy gradient of high-spin multiplet state calculated by the SAC-CI method. Chemical Physics Letters, 2001, 350, 351-358. | 1.2 | 16 |
| 128 | Theoretical investigation on the valence ionization spectra of Cl2O, ClOOCl, and F2O by correlation-based configuration interaction methods. Journal of Chemical Physics, 2003, 118, 5811-5820. | 1.2 | 16 |
| 129 | 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. | 1.2 | 16 |
| 130 | Electronic Transitions in Conformationally Controlled Peralkylated Hexasilanes. ChemPhysChem, 2016, 17, 3010-3022. | 1.0 | 16 |
| 131 | Coreâ€“Shell versus Other Structures in Binary Cu<sub>38â€“n</sub>M<sub>n</sub> 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. | 1.5 | 16 |
| 132 | Mechanism of NOâ€“CO reaction over highly dispersed cuprous oxide on Î³-alumina catalyst using a metalâ€“support interfacial site in the presence of oxygen: similarities to and differences from biological systems. Catalysis Science and Technology, 2018, 8, 3833-3845. | 2.1 | 16 |
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