

Yuriko Aoki

List of Publications by Year in descending order

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113
papers

1,595
citations

331670

21
h-index

377865

34
g-index

114
all docs

114
docs citations

114
times ranked

784
citing authors

#	ARTICLE	IF	CITATIONS
1	A theoretical synthesis of polymers by using uniform localization of molecular orbitals: Proposal of an elongation method. <i>Journal of Chemical Physics</i> , 1991, 95, 5419-5431.	3.0	159
2	A new localization scheme for the elongation method. <i>Journal of Chemical Physics</i> , 2004, 121, 10385-10391.	3.0	102
3	Local density of states of aperiodic polymers using the localized orbitals from an ab initio elongation method. <i>Journal of Chemical Physics</i> , 1992, 97, 8432-8440.	3.0	68
4	An elongation method for large systems toward bio-systems. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7640.	2.8	55
5	Elongation method with cutoff technique for linear SCF scaling. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 785-794.	2.0	46
6	Elongation method at restricted open-shell Hartree-Fock level of theory. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 875-882.	2.0	41
7	An efficient cluster elongation method in density functional theory and its application to polyhydrogen bonding molecules. <i>Journal of Chemical Physics</i> , 1994, 101, 10808-10823.	3.0	40
8	Synthesis of Monodispersedly Sized ZnO Nanowires from Randomly Sized Seeds. <i>Nano Letters</i> , 2020, 20, 599-605.	9.1	40
9	Efficiency and accuracy of the elongation method as applied to the electronic structures of large systems. <i>Journal of Computational Chemistry</i> , 2006, 27, 1603-1619.	3.3	35
10	Application of the elongation method to nonlinear optical properties: finite field approach for calculating static electric (hyper)polarizabilities. <i>Molecular Physics</i> , 2003, 101, 1487-1494.	1.7	33
11	Nonlinear optical properties of polydiacetylene with donor-acceptor substitution block. <i>Journal of Chemical Physics</i> , 2007, 127, 084702.	3.0	32
12	Investigation on the Electronic Structures and Nonlinear Optical Properties of Pristine Boron Nitride and Boron Nitride-Carbon Heterostructured Single-Wall Nanotubes by the Elongation Method. <i>Journal of Physical Chemistry C</i> , 2009, 113, 8447-8454.	3.1	32
13	Theoretical study on nonlinear optical properties of metalloporphyrin using elongation method. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 511-520.	1.4	31
14	Efficient and accurate calculations on the electronic structure of B-type poly(dG) TM poly(dC) DNA by elongation method: First step toward the understanding of the biological properties of aperiodic DNA. <i>Journal of Chemical Physics</i> , 2007, 126, 215104.	3.0	29
15	A simple rule to find nondisjoint NBMO degenerate systems for designing high-spin organic molecules. <i>International Journal of Quantum Chemistry</i> , 1999, 74, 491-502.	2.0	28
16	Dressed TDDFT study of low-lying electronic excited states in selected linear polyenes and diphenylopolynes. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 819-825.	2.0	27
17	Elongation cutoff technique armed with quantum fast multipole method for linear scaling. <i>Journal of Computational Chemistry</i> , 2009, 30, 2515-2525.	3.3	25
18	Investigation on nonlinear optical properties of ladder-structure polydiacetylenes derivatives by using the elongation finite-field method. <i>Chemical Physics Letters</i> , 2009, 474, 175-179.	2.6	25

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19	Electronic structures and nonlinear optical properties of supramolecular associations of benzo-2,1,3-chalcogendiazoles by the elongation method. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 453-460.	1.4	25
20	Helical molecular orbitals around straight-chain polyyne oligomers as models for molecular devices. <i>Chemical Physics Letters</i> , 2013, 590, 136-140.	2.6	25
21	Calculations of the excitation energies of all-trans and 11,12s-dicis retinals using localized molecular orbitals obtained by the elongation method. <i>Journal of Chemical Physics</i> , 1997, 107, 3569-3575.	3.0	24
22	A density functional elongation method for the theoretical synthesis of aperiodic polymers. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 267-280.	2.0	23
23	Rational Method of Monitoring Molecular Transformations on Metal-Oxide Nanowire Surfaces. <i>Nano Letters</i> , 2019, 19, 2443-2449.	9.1	21
24	Ab initio through space/bond interaction analysis on the stereoelectronic effect by modifying the exponents of the basis set. <i>International Journal of Quantum Chemistry</i> , 1999, 74, 761-768.	2.0	20
25	Band structures built by the elongation method. <i>Journal of Chemical Physics</i> , 2009, 130, 194106.	3.0	20
26	Calculations of the electronic structure of various aperiodic polymers by an elongation method. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 309-319.	2.0	19
27	Elongation cutoff technique at Kohn-Sham level of theory. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2130-2139.	2.0	19
28	Describing electron correlation effects in the framework of the elongation method—Elongation-MP2: Formalism, implementation and efficiency. <i>Journal of Computational Chemistry</i> , 2010, 31, 1733-1740.	3.3	18
29	Electronic structures of large, extended, nonperiodic systems by using the elongation method: Model calculations for the cluster series of a polymer and the molecular stacking on a surface. <i>International Journal of Quantum Chemistry</i> , 1995, 54, 167-196.	2.0	17
30	Analytical Method for Predicting Ferromagnetic Properties of Benzyl-Radical Polymers Based on NBMO Theory. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 786-796.	5.3	16
31	Theoretical Study of Cu Intercalation through a Defect in Zero-Layer Graphene on SiC Surface. <i>Journal of Physical Chemistry C</i> , 2017, 121, 7294-7302.	3.1	16
32	Calculations of phase transition of polydiacetylenes using localized molecular orbitals by elongation method. <i>Journal of Chemical Physics</i> , 1998, 108, 10303-10308.	3.0	15
33	NBO-based CI/MP through-space/bond interaction analysis and its application to stereoelectronic effects in SN2 reactions. <i>International Journal of Quantum Chemistry</i> , 2005, 104, 911-918.	2.0	15
34	Highly accurate O(N) method for delocalized systems. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 595-608.	1.4	15
35	Ab Initio MO Analysis of Interaction Paths between Radicals in Ferromagnetic Organic Systems. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5803-5808.	2.5	14
36	Extraction of One-Handed Helical Frontier Orbital in Even [<i>n</i>]Cumulenes by Breaking Mirror Images of Right- and Left-Handed Helical Orbitals: Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 11134-11139.	3.1	14

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37	Molecular and electronic structures of bipolaron in poly-para-phenylene in terms of molecular orbital symmetry. <i>Theoretical Chemistry Accounts</i> , 1999, 102, 180-187.	1.4	13
38	Performance of the elongation method with larger basis sets. <i>International Journal of Quantum Chemistry</i> , 1999, 74, 35-47.	2.0	13
39	Ab initio through-space/bond interaction analysis of the long C-C bonds in Bi(anthracene-9,10-dimethylene) photoisomers. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 456-467.	2.0	13
40	Application of the elongation method to the electronic structure of spin-polarized molecular wire under electric field. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 493-501.	1.4	13
41	Enhanced hyperpolarizability via electron correlations in donor- π -acceptor systems. <i>Physical Review A</i> , 2003, 68, .	2.5	12
42	Elongation method for calculating excited states of aromatic molecules embedded in polymers. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1328-1340.	2.0	12
43	Electronic structures and molecular structures of polyynes. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 423-427.	2.0	12
44	Three dimensional elongation method for large molecular calculations. <i>Chemical Physics Letters</i> , 2013, 560, 66-70.	2.6	12
45	Role of Pyridinium Groups and Iodide Ions in Photoelectrochromism in Viologen-Based Ion-Pair Charge-Transfer Complexes: Molecular Orbital Analysis. <i>Journal of Physical Chemistry C</i> , 2018, 122, 4546-4556.	3.1	12
46	Face-selective tungstate ions drive zinc oxide nanowire growth direction and dopant incorporation. <i>Communications Materials</i> , 2020, 1, .	6.9	12
47	Molecular design of a π -conjugated single-chain electronically conductive polymer. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1924-1933.	2.0	11
48	Linear-scaled excited state calculations at linear response time-dependent Hartree-Fock theory. <i>Molecular Physics</i> , 2010, 108, 205-210.	1.7	11
49	Counterion effects of A-type and B-type poly(dG)-Poly(dC) and poly(dA)-Poly(dT) DNA by elongation method. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 230-239.	2.0	11
50	A modified localization scheme for the three-dimensional elongation method applied to large systems. <i>Chemical Physics Letters</i> , 2013, 565, 143-147.	2.6	11
51	Development of minimized mixing molecular orbital method for designing organic ferromagnets. <i>Journal of Computational Chemistry</i> , 2015, 36, 1232-1239.	3.3	11
52	A thermally robust and strongly oxidizing surface of WO ₃ hydrate nanowires for electrical aldehyde sensing with long-term stability. <i>Journal of Materials Chemistry A</i> , 2021, 9, 5815-5824.	10.3	11
53	Electronic states of mixed base pairs systems of dna and the effect of base composition and sequences on the band structures using screw axis translational symmetry. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 489-496.	2.0	10
54	Pure through-bond state in organic molecules for analysis of the relationship between intramolecular interactions and total energy. <i>International Journal of Quantum Chemistry</i> , 2003, 92, 355-366.	2.0	9

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55	Elongation method and supermolecule approach for the calculation of nonlinear susceptibilities. Application to the 3-Methyl-4-Nitropyridine 1-Oxide and 2-Methyl-4-Nitroaniline crystals. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2006, 6, 171-188.	0.2	9
56	Electronic properties of tricoordinated phosphorus in hexagonal phosphinium compounds and molecular aromaticity. <i>Journal of Computational Chemistry</i> , 2007, 28, 1467-1475.	3.3	9
57	Geometry optimization for large systems by the elongation method. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	9
58	Ab initio O(N) elongation-counterpoise method for BSSE-corrected interaction energy analyses in biosystems. <i>Journal of Chemical Physics</i> , 2015, 142, 104111.	3.0	9
59	One-Handed Helical Orbitals in Conjugated Molecules. <i>ACS Central Science</i> , 2018, 4, 664-665.	11.3	9
60	Perturbational approach to aperiodicity of polymer systems. <i>International Journal of Quantum Chemistry</i> , 1987, 32, 137-151.	2.0	8
61	Substituent Effects on Menshutkin-Type Reactions in the Gas Phase and Solutions: Theoretical Approach from the Orbital Interaction View. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4035-4045.	5.3	8
62	Molecular orbital approach to the Peierls instability in polyenes and its application to model crystals of charge-transfer complexes. <i>International Journal of Quantum Chemistry</i> , 1997, 64, 325-336.	2.0	7
63	Quantum-chemical approach to the solvatochromic transition in polysilane derivatives. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2006, 44, 119-133.	2.1	7
64	An Efficient Local Molecular Dynamics Polymerization Simulation Combined with an Ab Initio MO Method. <i>Materials</i> , 2013, 6, 870-885.	2.9	7
65	Theoretical synthesis of poly-(2-hydroxyethylmethacrylate) by uniform localization of molecular orbitals calculation. <i>Journal of Polymer Science Part A</i> , 2001, 39, 2677-2682.	2.3	6
66	Theoretical study on static (hyper)polarizabilities for polyimide by the elongation finite-field method. <i>Molecular Physics</i> , 2009, 107, 81-87.	1.7	6
67	Elongation method for electronic structure calculations of random DNA sequences. <i>Journal of Computational Chemistry</i> , 2015, 36, 2103-2113.	3.3	6
68	Nonlinear optical properties of push-pull systems containing [2.2]paracyclophane: Theoretical study via elongation method. <i>Chemical Physics Letters</i> , 2020, 755, 137760.	2.6	6
69	An analytical molecular orbital approach for modeling of low-dimensional conductors in molecular crystals. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 401-415.	2.0	5
70	An analytical molecular orbital approach in tetrathiafulvalene tetracyanoquinodimethane (TTF-TCNQ). <i>Molecular Physics</i> , 2004, 102, 1891-1901.	1.7	5
71	Elongation method for linear scaling SCF calculations of polymers. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2006, 6, 189-200.	0.2	5
72	Guidelines proposed for designing organic ferromagnets by using a quantum chemical approach. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 789-806.	1.4	5

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73	An Analytical Approach to Predict High-spin Stability of Conjugated Hydrocarbon Radical Polymers using Minimized Mixing Nonbonding Molecular Orbitals. <i>Current Physical Chemistry</i> , 2013, 3, 99-112.	0.2	5
74	Why does 2-(2-aminoethylamino)ethanol have superior CO ₂ separation performance to monoethanolamine? A computational study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14172-14176.	2.8	5
75	Novel-Type Charge-Transfer Complex Formation between Indoxyl Sulfate and Anthraquinonesulfonate Ions in an Aqueous Polyelectrolyte Solution. <i>Polymer Journal</i> , 2003, 35, 50-55.	2.7	4
76	Stereoelectronic effects in Menshutkin-type S _N 2 reactions: theoretical study based on through-space/bond orbital interaction analysis. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 885-891.	1.9	4
77	Automated property optimization via ab initio O(N) elongation method: Application to (hyper-)polarizability in DNA. <i>Journal of Chemical Physics</i> , 2016, 145, 024107.	3.0	4
78	Quantum chemistry-machine learning approach for predicting and elucidating molecular hyperpolarizability: Application to [2.2]paracyclophane-containing push-pull polymers. <i>Journal of Chemical Physics</i> , 2021, 154, 124107.	3.0	4
79	Computational approach for investigating the mechanism of carbon dioxide interaction by 2-(2-aminoethylamino)ethanol: A significant role of water molecule. <i>Chemical Physics Letters</i> , 2021, 783, 139070.	2.6	4
80	ELONGATION METHOD FOR POLYMERS AND ITS APPLICATION TO NONLINEAR OPTICS. , 2006, , 97-177.		3
81	Elongation-CIS method: Describing excited states of large molecular systems in regionally localized molecular orbital basis. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2010, 10, 473-481.	0.2	3
82	Intermediate electrostatic field for the elongation method. <i>Journal of Molecular Modeling</i> , 2014, 20, 2277.	1.8	3
83	Efficient prediction of high spin ground state stability in organic polyradicals under solvent effects. <i>Chemical Physics Letters</i> , 2015, 637, 143-147.	2.6	3
84	Intermediate Electrostatic Field for the Generalized Elongation Method. <i>ChemPhysChem</i> , 2015, 16, 1551-1556.	2.1	3
85	Interaction of OH [•] with xylan and its hydrated complexes: structures and molecular dynamics study using elongation method. <i>Journal of Molecular Modeling</i> , 2015, 21, 117.	1.8	3
86	Importance of Through-Space Interaction of [2,2]-Paracyclophane-oligo(<i>p</i> -phenylenevinylene) Molecular Wires for Photovoltaic Application and Effective Wire Design by Chemical Substitution. <i>Journal of Physical Chemistry C</i> , 2017, 121, 17703-17711.	3.1	3
87	Ab initio multi-level layered elongation method and its application to local interaction analysis between DNA bulge and ligand molecules. <i>Journal of Chemical Physics</i> , 2021, 155, 044110.	3.0	3
88	Molecular Orbital Study on the Ferroelectricity of Odd Nylons. <i>Molecular Crystals and Liquid Crystals</i> , 1996, 278, 99-109.	0.3	2
89	Generalized elongation method: From one-dimension to three-dimension. , 2012, , .		2
90	Development of molecular fragment interaction method for designing organic ferromagnets. <i>Journal of Mathematical Chemistry</i> , 2016, 54, 1585-1595.	1.5	2

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91	An Efficient Unrestricted PCM-Elongation Method for Large High-Spin Polymer/Dendrimer Systems. <i>Zeitschrift Fur Physikalische Chemie</i> , 2016, 230, 667-680.	2.8	2
92	An attempt at ab initio crystal orbital calculation of electronic structure of B-type model-DNA. <i>AIP Conference Proceedings</i> , 2017, , .	0.4	2
93	Microscopic Hopping Mechanism of an Isolated PTCDA Molecule on a Reactive Ge(001) Surface. <i>Journal of Physical Chemistry C</i> , 2020, 124, 24704-24712.	3.1	2
94	Important role of Si main chain for solvatochromism in poly[bis(4-propoxybutyl)silylene]. <i>Journal of Polymer Science Part A</i> , 2003, 41, 483-486.	2.3	1
95	Band Structure of Polymer Extracted from Oligomer Calculations. <i>AIP Conference Proceedings</i> , 2007, , .	0.4	1
96	Band structure of polymer extracted from oligomer calculations by elongation method and its applications to nanosystems. , 2012, , .		1
97	Efficient algorithm for computing orbital energies within elongation method. , 2012, , .		1
98	Computational scheme to determine local vibrations of large systems using elongation method. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	1.4	1
99	Elongation method with intermediate mechanical and electrostatic embedding for geometry optimizations of polymers. <i>Journal of Computational Chemistry</i> , 2020, 41, 2203-2212.	3.3	1
100	Theoretical Analysis of Properties of Ground and Excited States for Photodissociation of the C=O Bond in Polycarbonates. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6662-6673.	2.5	1
101	Ab initio through-space/bond interaction analysis of the long C-C bonds in Bi(anthracene-9,10-dimethylene) photoisomers. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 456.	2.0	1
102	Efficient analytical approach for predicting the Peierls distortion in molecular crystals. <i>Physical Review B</i> , 2008, 77, .	3.2	0
103	A Festschrift in honor of Sándor Suhai's 65th birthday. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 101-105.	1.4	0
104	A Festschrift in honor of Akira Imamura's 77th birthday, his recent retirement, and his many contributions to theoretical chemistry. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 571-574.	1.4	0
105	Elongation method for linear scaling. , 2012, , .		0
106	Reply to the comment of J. Ladik on "electronic states of mixed base pairs systems of DNA and the effect of base composition and sequences on the band structures using screw axis translational symmetry". <i>International Journal of Quantum Chemistry</i> , 2014, 114, 303-303.	2.0	0
107	Computational Study of Cu-Containing Artificial DNA: Twist Angle Dependence of Magnetism. <i>ChemistrySelect</i> , 2016, 1, 5521-5529.	1.5	0
108	Ab initio electronic structure calculation of polymononucleotide, a model of B-type DNA. <i>AIP Conference Proceedings</i> , 2018, , .	0.4	0

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109	Extent of structural change during the reaction and its relationship to isoselectivity in polypropylene polymerization with ansa η -Zirconocene/borate catalyst: A computational study. <i>Journal of Computational Chemistry</i> , 2019, 40, 2622-2635.	3.3	0
110	Through-Space/Bond Interaction Analysis of Ferromagnetic Interactions. <i>Springer Briefs in Molecular Science</i> , 2017, , 101-120.	0.1	0
111	O(N) Ab Initio Open-Shell MMELG-PCM Method and Its Application to Radical Polymers. <i>Springer Briefs in Molecular Science</i> , 2017, , 121-135.	0.1	0
112	Nonbonding Molecular Orbital Method and Mathematical Proof for Disjoint/Non-disjoint Molecules. <i>Springer Briefs in Molecular Science</i> , 2017, , 31-59.	0.1	0
113	Local electronic structure analysis by ab initio elongation method: a benchmark using DNA block polymers. <i>Journal of Chemical Physics</i> , 0, , .	3.0	0