Yuriko Aoki

List of Publications by Year
in descending order

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	Why does 2-(2-aminoethylamino)ethanol have superior CO₂ separation performance to monoethanolamine? A computational study. Physical Chemistry Chemical Physics, 2022, 24, 14172-14176.	2.8	5
2	Quantum chemistryâ€“machine learning approach for predicting and elucidating molecular hyperpolarizability: Application to [2.2]paracyclophane-containing pushâ€“pull polymers. Journal of Chemical Physics, 2021, 154, 124107.	3.0	4
3	Theoretical Analysis of Properties of Ground and Excited States for Photodissociation of the Câ€“O Bond in Polycarbonates. Journal of Physical Chemistry A, 2021, 125, 6662-6673.	2.5	1
4	Ab initio multi-level layered elongation method and its application to local interaction analysis between DNA bulge and ligand molecules. Journal of Chemical Physics, 2021, 155, 044110.	3.0	3
5	Computational approach for investigating the mechanism of carbon dioxide interaction by 2-(2-aminoethylamino)ethanol: A significant role of water molecule. Chemical Physics Letters, 2021, 783, 139070.	2.6	4
6	A thermally robust and strongly oxidizing surface of WO₃hydrate nanowires for electrical aldehyde sensing with long-term stability. Journal of Materials Chemistry A, 2021, 9, 5815-5824.	10.3	11
7	Synthesis of Monodispersedly Sized ZnO Nanowires from Randomly Sized Seeds. Nano Letters, 2020, 20, 599-605.	9.1	40
8	Nonlinear optical properties of push-pull systems containing [2.2]paracyclophane: Theoretical study via elongation method. Chemical Physics Letters, 2020, 755, 137760.	2.6	6
9	Microscopic Hopping Mechanism of an Isolated PTCDA Molecule on a Reactive Ge(001) Surface. Journal of Physical Chemistry C, 2020, 124, 24704-24712.	3.1	2
10	Elongation method with intermediate mechanical and electrostatic embedding for geometry optimizations of polymers. Journal of Computational Chemistry, 2020, 41, 2203-2212.	3.3	1
11	Face-selective tungstate ions drive zinc oxide nanowire growth direction and dopant incorporation. Communications Materials, 2020, 1, .	6.9	12
12	Extent of structural change during the reaction and its relationship to isoselectivity in polypropylene polymerization with ansa â€zirconocene/borate catalyst: A computational study. Journal of Computational Chemistry, 2019, 40, 2622-2635.	3.3	0
13	Rational Method of Monitoring Molecular Transformations on Metal-Oxide Nanowire Surfaces. Nano Letters, 2019, 19, 2443-2449.	9.1	21
14	Extraction of One-Handed Helical Frontier Orbital in Even [n]Cumulenes by Breaking Mirror Images of Right- and Left-Handed Helical Orbitals: Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 11134-11139.	3.1	14
15	Role of Pyridinium Groups and Iodide Ions in Photoelectrochromism in Viologen-Based Ion-Pair Charge-Transfer Complexes: Molecular Orbital Analysis. Journal of Physical Chemistry C, 2018, 122, 4546-4556.	3.1	12
16	Ab initio electronic structure calculation of polymononucleotide, a model of B-type DNA. AIP Conference Proceedings, 2018, , .	0.4	0
17	One-Handed Helical Orbitals in Conjugated Molecules. ACS Central Science, 2018, 4, 664-665.	11.3	9
18	Theoretical Study of Cu Intercalation through a Defect in Zero-Layer Graphene on SiC Surface. Journal of Physical Chemistry C, 2017, 121, 7294-7302.	3.1	16

#	Article	IF	Citations
19	Computational scheme to determine local vibrations of large systems using elongation method. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	1
20	Importance of Through-Space Interaction of [2,2â€²]-Paracyclophane-oligo(p-phenylenevinylene) Molecular Wires for Photovoltaic Application and Effective Wire Design by Chemical Substitution. Journal of Physical Chemistry C, 2017, 121, 17703-17711.	3.1	3
21	An attempt at ab initio crystal orbital calculation of electronic structure of B-type model-DNA. AIP Conference Proceedings, 2017, , .	0.4	2
22	Through-Space/Bond Interaction Analysis of Ferromagnetic Interactions. Springer Briefs in Molecular Science, 2017, , 101-120.	0.1	0
23	O(N) Ab Initio Open-Shell MMELG-PCM Method and Its Application to Radical Polymers. Springer Briefs in Molecular Science, 2017, , 121-135.	0.1	0
24	Nonbonding Molecular Orbital Method and Mathematical Proof for Disjoint/Non-disjoint Molecules. Springer Briefs in Molecular Science, 2017, , 31-59.	0.1	0
25	Automated property optimization via ab initio O(N) elongation method: Application to (hyper-)polarizability in DNA. Journal of Chemical Physics, 2016, 145, 024107.	3.0	4
26	Computational Study of Cuâ€“Containing Artificial DNA: Twist Angle Dependence of Magnetism. ChemistrySelect, 2016, 1, 5521-5529.	1.5	0
27	Development of molecular fragment interaction method for designing organic ferromagnets. Journal of Mathematical Chemistry, 2016, 54, 1585-1595.	1.5	2
28	An Efficient Unrestricted PCM-Elongation Method for Large High-Spin Polymer/Dendrimer Systems. Zeitschrift Fur Physikalische Chemie, 2016, 230, 667-680.	2.8	2
29	Efficient prediction of high spin ground state stability in organic polyradicals under solvent effects. Chemical Physics Letters, 2015, 637, 143-147.	2.6	3
30	Intermediate Electrostatic Field for the Generalized Elongation Method. ChemPhysChem, 2015, 16, 1551-1556.	2.1	3
31	Elongation method for electronic structure calculations of random DNA sequences. Journal of Computational Chemistry, 2015, 36, 2103-2113.	3.3	6
32	Development of minimized mixing molecular orbital method for designing organic ferromagnets. Journal of Computational Chemistry, 2015, 36, 1232-1239.	3.3	11
33	Interaction of OHâ˜ with xylan and its hydrated complexes: structures and molecular dynamics study using elongation method. Journal of Molecular Modeling, 2015, 21, 117.	1.8	3
34	Ab initio O(N) elongation-counterpoise method for BSSE-corrected interaction energy analyses in biosystems. Journal of Chemical Physics, 2015, 142, 104111.	3.0	9
35	Reply to the comment of J. Ladik on â€œelectronic states of mixed base pairs systems of DNA and the effect of base composition and sequences on the band structures using screw axis translational symmetryâ€• International Journal of Quantum Chemistry, 2014, 114, 303-303.	2.0	0
36	Intermediate electrostatic field for the elongation method. Journal of Molecular Modeling, 2014, 20, 2277.	1.8	3

#	Article	IF	Citations
37	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. International Journal of Quantum Chemistry, 2013, 113, 489-496.	2.0	10
38	Electronic structures and molecular structures of polyynes. International Journal of Quantum Chemistry, 2013, 113, 423-427.	2.0	12
39	Helical molecular orbitals around straight-chain polyyne oligomers as models for molecular devices. Chemical Physics Letters, 2013, 590, 136-140.	2.6	25
40	Substituent Effects on Menshutkin-Type Reactions in the Gas Phase and Solutions: Theoretical Approach from the Orbital Interaction View. Journal of Chemical Theory and Computation, 2013, 9, 4035-4045.	5.3	8
41	A modified localization scheme for the three-dimensional elongation method applied to large systems. Chemical Physics Letters, 2013, 565, 143-147.	2.6	11
42	Three dimensional elongation method for large molecular calculations. Chemical Physics Letters, 2013, 560, 66-70.	2.6	12
43	Stereoelectronic effects in Menshutkinâ€type S_N2 reactions: theoretical study based on throughâ€space/bond orbital interaction analysis. Journal of Physical Organic Chemistry, 2013, 26, 885-891.	1.9	4
44	An Efficient Local Molecular Dynamics Polymerization Simulation Combined with an Ab Initio MO Method. Materials, 2013, 6, 870-885.	2.9	7
45	An Analytical Approach to Predict High-spin Stability of Conjugated Hydrocarbon Radical Polymers using Minimized Mixing Nonbonding Molecular Orbitals. Current Physical Chemistry, 2013, 3, 99-112.	0.2	5
46	Band structure of polymer extracted from oligomer calculations by elongation method and its applications to nanosystems. , 2012, , .		1
47	Generalized elongation method: From one-dimension to three-dimension. , 2012, , .		2
48	Geometry optimization for large systems by the elongation method. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	9
49	An elongation method for large systems toward bio-systems. Physical Chemistry Chemical Physics, 2012, 14, 7640.	2.8	55
50	Efficient algorithm for computing orbital energies within elongation method. , 2012, , .		1
51	Elongation method for linear scaling. , 2012, , .		0
52	Counterâ€ion effects of Aâ€•and Bâ€type poly(dG)·Poly(dC) and poly(dA)·Poly(dT) DNA by elongation method. International Journal of Quantum Chemistry, 2012, 112, 230-239.	2.0	11
53	Highly accurate O(N) method for delocalized systems. Theoretical Chemistry Accounts, 2011, 130, 595-608.	1.4	15
54	A Festschrift in honor of Akira Imamuraâ€™s 77th birthday, his recent retirement, and his many contributions to theoretical chemistry. Theoretical Chemistry Accounts, 2011, 130, 571-574.	1.4	0

#	Article	IF	Citations
55	Guidelines proposed for designing organic ferromagnets by using a quantum chemical approach. Theoretical Chemistry Accounts, 2011, 130, 789-806.	1.4	5
56	Dressed TDDFT study of lowâ€lying electronic excited states in selected linear polyenes and diphenylopolyenes. International Journal of Quantum Chemistry, 2011, 111, 819-825.	2.0	27
57	Describing electron correlation effects in the framework of the elongation methodâ€"Elongationâ€MP2: Formalism, implementation and efficiency. Journal of Computational Chemistry, 2010, 31, 1733-1740.	3.3	18
58	Electronic structures and nonlinear optical properties of supramolecular associations of benzo-2,1,3-chalcogendiazoles by the elongation method. Theoretical Chemistry Accounts, 2010, 125, 453-460.	1.4	25
59	Application of the elongation method to the electronic structure of spin-polarized molecular wire under electric field. Theoretical Chemistry Accounts, 2010, 125, 493-501.	1.4	13
60	Theoretical study on nonlinear optical properties of metalloporphyrin using elongation method. Theoretical Chemistry Accounts, 2010, 125, 511-520.	1.4	31
61	A Festschrift in honor of SÃ¡ndor Suhaiâ€™s 65th birthday. Theoretical Chemistry Accounts, 2010, 125, 101-105.	1.4	0
62	Elongation cutoff technique at Kohnâ€“Sham level of theory. International Journal of Quantum Chemistry, 2010, 110, 2130-2139.	2.0	19
63	Elongation-CIS method: Describing excited states of large molecular systems in regionally localized molecular orbital basis. Journal of Computational Methods in Sciences and Engineering, 2010, 10, 473-481.	0.2	3
64	Linear-scaled excited state calculations at linear response time-dependent Hartreeâ€“Fock theory. Molecular Physics, 2010, 108, 205-210.	1.7	11
65	Elongation cutoff technique armed with quantum fast multipole method for linear scaling. Journal of Computational Chemistry, 2009, 30, 2515-2525.	3.3	25
66	Elongation method for calculating excited states of aromatic molecules embedded in polymers. International Journal of Quantum Chemistry, 2009, 109, 1328-1340.	2.0	12
67	Investigation on nonlinear optical properties of ladder-structure polydiacetylenes derivatives by using the elongation finite-field method. Chemical Physics Letters, 2009, 474, 175-179.	2.6	25
68	Band structures built by the elongation method. Journal of Chemical Physics, 2009, 130, 194106.	3.0	20
69	Investigation on the Electronic Structures and Nonlinear Optical Properties of Pristine Boron Nitride and Boron Nitrideâ"Carbon Heterostructured Single-Wall Nanotubes by the Elongation Method. Journal of Physical Chemistry C, 2009, 113, 8447-8454.	3.1	32
70	Theoretical study on static (hyper)polarizabilities for polyimide by the elongation finite-field method. Molecular Physics, 2009, 107, 81-87.	1.7	6
71	Efficient analytical approach for predicting the Peierls distortion in molecular crystals. Physical Review B, 2008, 77, .	3.2	0
72	Nonlinear optical properties of polydiacetylene with donor-acceptor substitution block. Journal of Chemical Physics, 2007, 127, 084702.	3.0	32

#	Article	IF	Citations
73	Band Structure of Polymer Extracted from Oligomer Calculations. AIP Conference Proceedings, 2007, , .	0.4	1
74	Efficient and accurate calculations on the electronic structure of B-type poly(dG)â^™poly(dC) DNA by elongation method: First step toward the understanding of the biological properties of aperiodic DNA. Journal of Chemical Physics, 2007, 126, 215104.	3.0	29
75	Electronic properties of tricoordinated phosphorus in hexagonal phosphininium compounds and molecular aromaticity. Journal of Computational Chemistry, 2007, 28, 1467-1475.	3.3	9
76	Analytical Method for Predicting Ferromagnetic Properties of Benzyl-Radical Polymers Based on NBMO Theory. Journal of Chemical Theory and Computation, 2006, 2, 786-796.	5.3	16
77	Ab Initio MO Analysis of Interaction Paths between Radicals in Ferromagnetic Organic Systems. Journal of Physical Chemistry A, 2006, 110, 5803-5808.	2.5	14
78	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. Journal of Computational Methods in Sciences and Engineering, 2006, 6, 171-188.	0.2	9
79	Elongation method for linear scaling SCF calculations of polymers. Journal of Computational Methods in Sciences and Engineering, 2006, 6, 189-200.	0.2	5
80	ELONGATION METHOD FOR POLYMERS AND ITS APPLICATION TO NONLINEAR OPTICS. , 2006, , 97-177.		3
81	Molecular design of a Ï€-conjugated single-chain electronically conductive polymer. International Journal of Quantum Chemistry, 2006, 106, 1924-1933.	2.0	11
82	Quantum-chemical approach to the solvatochromic transition in polysilane derivatives. Journal of Polymer Science, Part B: Polymer Physics, 2006, 44, 119-133.	2.1	7
83	Efficiency and accuracy of the elongation method as applied to the electronic structures of large systems. Journal of Computational Chemistry, 2006, 27, 1603-1619.	3.3	35
84	Elongation method with cutoff technique for linear SCF scaling. International Journal of Quantum Chemistry, 2005, 102, 785-794.	2.0	46
85	NBO-based CI/MP through-space/bond interaction analysis and its application to stereoelectronic effects in SN2 reactions. International Journal of Quantum Chemistry, 2005, 104, 911-918.	2.0	15
86	Elongation method at restricted open-shell Hartree-Fock level of theory. International Journal of Quantum Chemistry, 2005, 105, 875-882.	2.0	41
87	A new localization scheme for the elongation method. Journal of Chemical Physics, 2004, 121, 10385-10391.	3.0	102
88	An analytical molecular orbital approach in tetrathiafulvalene tetracyanoquinodimethane (TTF-TCNQ). Molecular Physics, 2004, 102, 1891-1901.	1.7	5
89	Important role of Si main chain for solvatochromism in poly[bis(4-propoxybutyl)silylene]. Journal of Polymer Science Part A, 2003, 41, 483-486.	2.3	1
90	Pure through-bond state in organic molecules for analysis of the relationship between intramolecular interactions and total energy. International Journal of Quantum Chemistry, 2003, 92, 355-366.	2.0	9

#	Article	IF	Citations
91	Enhanced hyperpolarizability via electron correlations in donor-Ïƒ-acceptor systems. Physical Review A, 2003, 68, .	2.5	12
92	Application of the elongation method to nonlinear optical properties: finite field approach for calculating static electric (hyper)polarizabilities. Molecular Physics, 2003, 101, 1487-1494.	1.7	33
93	Novel-Type Charge-Transfer Complex Formation between Indoxyl Sulfate and Anthraquinonesulfonate Ions in an Aqueous Polyelectrolyte Solution. Polymer Journal, 2003, 35, 50-55.	2.7	4
94	An analytical molecular orbital approach for modeling of low-dimensional conductors in molecular crystals. International Journal of Quantum Chemistry, 2002, 86, 401-415.	2.0	5
95	Ab initio through-space/bond interaction analysis of the long C-C bonds in Bi(anthracene-9,10-dimethylene) photoisomers. International Journal of Quantum Chemistry, 2002, 86, 456-467.	2.0	13
96	Ab initio through-space/bond interaction analysis of the long Câ€“C bonds in Bi(anthracene-9,10-dimethylene) photoisomers. International Journal of Quantum Chemistry, 2002, 86, 456.	2.0	1
97	Theoretical synthesis of poly-(2-hydroxyethylmethacrylate) by uniform localization of molecular orbitals calculation. Journal of Polymer Science Part A, 2001, 39, 2677-2682.	2.3	6
98	Molecular and electronic structures of bipolaron in poly-para-phenylene in terms of molecular orbital symmetry. Theoretical Chemistry Accounts, 1999, 102, 180-187.	1.4	13
99	Performance of the elongation method with larger basis sets. International Journal of Quantum Chemistry, 1999, 74, 35-47.	2.0	13
100	A simple rule to find nondisjoint NBMO degenerate systems for designing high-spin organic molecules. International Journal of Quantum Chemistry, 1999, 74, 491-502.	2.0	28
101	Ab initio through space/bond interaction analysis on the stereoelectronic effect by modifying the exponents of the basis set. International Journal of Quantum Chemistry, 1999, 74, 761-768.	2.0	20
102	Calculations of phase transition of polydiacetylenes using localized molecular orbitals by elongation method. Journal of Chemical Physics, 1998, 108, 10303-10308.	3.0	15
103	Calculations of the excitation energies of all-trans and 11,12s-dicis retinals using localized molecular orbitals obtained by the elongation method. Journal of Chemical Physics, 1997, 107, 3569-3575.	3.0	24
104	Molecular orbital approach to the Peierls instability in polyenes and its application to model crystals of charge-transfer complexes. International Journal of Quantum Chemistry, 1997, 64, 325-336.	2.0	7
105	Molecular Orbital Study on the Ferroelectricity of Odd Nylons. Molecular Crystals and Liquid Crystals, 1996, 278, 99-109.	0.3	2
106	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. International Journal of Quantum Chemistry, 1995, 54, 167-196.	2.0	17
107	An efficient cluster elongation method in density functional theory and its application to polyâ€hydrogenâ€bonding molecules. Journal of Chemical Physics, 1994, 101, 10808-10823.	3.0	40
108	A density functional elongation method for the theoretical synthesis of aperiodic polymers. International Journal of Quantum Chemistry, 1994, 52, 267-280.	2.0	23

#	Article	IF	Citations
109	Calculations of the electronic structure of various aperiodic polymers by an elongation method. International Journal of Quantum Chemistry, 1994, 52, 309-319.	2.0	19
110	Local density of states of aperiodic polymers using the localized orbitals from anab initioelongation method. Journal of Chemical Physics, 1992, 97, 8432-8440.	3.0	68
111	A theoretical synthesis of polymers by using uniform localization of molecular orbitals: Proposal of an elongation method. Journal of Chemical Physics, 1991, 95, 5419-5431.	3.0	159
112	Perturbational approach to aperiodicity of polymer systems. International Journal of Quantum Chemistry, 1987, 32, 137-151.	2.0	8
113	Local electronic structure analysis by ab initio elongation method: a benchmark using DNA block polymers. Journal of Chemical Physics, 0, , .	3.0	0