Hiromi Nakai

List of Publications by Year
in descending order

344 papers	8,542 citations	57719 44 h-index	79644 73 g-index
350 all docs	350 docs citations	350 times ranked	5894 citing authors

#	Article	IF	Citations
1	Theoretical Analysis of Interactions between Potassium Ions and Organic Electrolyte Solvents: A Comparison with Lithium, Sodium, and Magnesium Ions. Journal of the Electrochemical Society, 2017, 164, A54-A60.	1.3	276
2	Unveiling a New Aspect of Simple Arylboronic Esters: Long-Lived Room-Temperature Phosphorescence from Heavy-Atom-Free Molecules. Journal of the American Chemical Society, 2017, 139, 2728-2733.	6.6	269
3	Theoretical Analysis on De-Solvation of Lithium, Sodium, and Magnesium Cations to Organic Electrolyte Solvents. Journal of the Electrochemical Society, 2013, 160, A2160-A2165.	1.3	227
4	An extension of ab initio molecular orbital theory to nuclear motion. Chemical Physics Letters, 1998, 290, 437-442.	1.2	209
5	Density functional method including weak interactions: Dispersion coefficients based on the local response approximation. Journal of Chemical Physics, 2009, 131, 224104.	1.2	204
6	Alternative linear-scaling methodology for the second-order MÃ¸ller-Plesset perturbation calculation based on the divide-and-conquer method. Journal of Chemical Physics, 2007, 127, 074103.	1.2	141
7	Extension of linear-scaling divide-and-conquer-based correlation method to coupled cluster theory with singles and doubles excitations. Journal of Chemical Physics, 2008, 129, 044103.	1.2	135
8	Implementation of divide-and-conquer method including Hartree-Fock exchange interaction. Journal of Computational Chemistry, 2007, 28, 2003-2012.	1.5	130
9	Energy density analysis with Kohnâ€“Sham orbitals. Chemical Physics Letters, 2002, 363, 73-79.	1.2	126
10	Divide-and-conquer-based linear-scaling approach for traditional and renormalized coupled cluster methods with single, double, and noniterative triple excitations. Journal of Chemical Physics, 2009, 131, 114108.	1.2	126
11	Simultaneous determination of nuclear and electronic wave functions without Born-Oppenheimer approximation: Ab initio NO+MO/HF theory. International Journal of Quantum Chemistry, 2002, 86, 511-517.	1.0	116
12	Confined water-mediated high proton conduction in hydrophobic channel of a synthetic nanotube. Nature Communications, 2020, 11, 843.	5.8	116
13	Many-body effects in nonadiabatic molecular theory for simultaneous determination of nuclear and electronic wave functions:Ab initioNOMO/MBPT and CC methods. Journal of Chemical Physics, 2003, 118, 1119-1127.	1.2	96
14	Local response dispersion method. II. Generalized multicenter interactions. Journal of Chemical Physics, 2010, 133, 194101.	1.2	89
15	Nuclear orbital plus molecular orbital theory: Simultaneous determination of nuclear and electronic wave functions without Bornâ€“Oppenheimer approximation. International Journal of Quantum Chemistry, 2007, 107, 2849-2869.	1.0	88
16	Three pillars for achieving quantum mechanical molecular dynamics simulations of huge systems: Divideâ€andâ€conquer, densityâ€functional tightâ€binding, and massively parallel computation. Journal of Computational Chemistry, 2016, 37, 1983-1992.	1.5	88
17	Sodiumâ€and Potassiumâ€Hydrate Melts Containing Asymmetric Imide Anions for Highâ€Voltage Aqueous Batteries. Angewandte Chemie - International Edition, 2019, 58, 14202-14207.	7.2	81
18	Ab initio molecular orbital model of scanning tunneling microscopy. Journal of Chemical Physics, 1996, 104, 2410-2417.	1.2	80

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19	Local unitary transformation method for large-scale two-component relativistic calculations: Case for a one-electron Dirac Hamiltonian. Journal of Chemical Physics, 2012, 136, 244102.	1.2	76
20	Reversible Sodium Metal Electrodes: Is Fluorine an Essential Interphasial Component?. Angewandte Chemie - International Edition, 2019, 58, 8024-8028.	7.2	76
21	Dipped adcluster model study for molecular and dissociative chemisorptions of O2 on Ag surface. Journal of Chemical Physics, 1993, 98, 2423-2436.	1.2	75
22	Time-dependent density functional theory calculations for core-excited states: Assessment of standard exchange-correlation functionals and development of a novel hybrid functional. Journal of Chemical Physics, 2006, 124, 094105.	1.2	73
23	Second-order MÃ¸ller-Plesset perturbation energy obtained from divide-and-conquer Hartree-Fock density matrix. Journal of Chemical Physics, 2006, 125, 204106.	1.2	72
24	Molecular orbital study on the reaction process of dimethylamine borane as a reductant for electroless deposition. Journal of Electroanalytical Chemistry, 2003, 559, 131-136.	1.9	70
25	How does it become possible to treat delocalized and/or open-shell systems in fragmentation-based linear-scaling electronic structure calculations? The case of the divide-and-conquer method. Physical Chemistry Chemical Physics, 2012, 14, 7629.	1.3	68
26	Theoretical Analysis of Carrier Ion Diffusion in Superconcentrated Electrolyte Solutions for Sodium-Ion Batteries. Journal of Physical Chemistry B, 2018, 122, 2600-2609.	1.2	67
27	Semi-local machine-learned kinetic energy density functional with third-order gradients of electron density. Journal of Chemical Physics, 2018, 148, 241705.	1.2	67
28	Hybrid exchange-correlation functional for core, valence, and Rydberg excitations: Core-valence-Rydberg B3LYP. Journal of Chemical Physics, 2006, 125, 064109.	1.2	65
29	Non-Bornâ€“Oppenheimer theory for simultaneous determination of vibrational and electronic excited states: ab initio NO+MO/CIS theory. Chemical Physics Letters, 2001, 345, 118-124.	1.2	64
30	Activation of O2 on Cu, Ag, and Au surfaces for the epoxidation of ethylene: dipped adcluster model study. Surface Science, 1997, 387, 328-341.	0.8	63
31	Elimination of translational and rotational motions in nuclear orbital plus molecular orbital theory. Journal of Chemical Physics, 2005, 122, 164101.	1.2	63
32	Molecular orbital study on the reaction mechanisms of electroless deposition processes. Electrochimica Acta, 2001, 47, 47-53.	2.6	62
33	Dualâ€level hierarchical scheme for linearâ€scaling divideâ€andâ€conquer correlation theory. International Journal of Quantum Chemistry, 2009, 109, 2227-2237.	1.0	61
34	Theoretical study on the ground and excited states of MnOâ¯4. Journal of Chemical Physics, 1991, 95, 8287-8291.	1.2	58
35	D<scp>cdftbmd</scp>: Divideâ€andâ€Conquer Density Functional Tightâ€Binding Program for Hugeâ€System Quantum Mechanical Molecular Dynamics Simulations. Journal of Computational Chemistry, 2019, 40, 1538-1549.	1.5	58
36	Assessment of self-consistent field convergence in spin-dependent relativistic calculations. Chemical Physics Letters, 2016, 657, 65-71.	1.2	55

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37	Generalized MÃ¸llerâ€“Plesset Partitioning in Multiconfiguration Perturbation Theory. Journal of Chemical Theory and Computation, 2010, 6, 2024-2033.	2.3	53
38	Divide-and-Conquer-Type Density-Functional Tight-Binding Molecular Dynamics Simulations of Proton Diffusion in a Bulk Water System. Journal of Physical Chemistry B, 2016, 120, 217-221.	1.2	53
39	Catalytic performance of Ru, Os, and Rh nanoparticles for ammonia synthesis: A density functional theory analysis. Journal of Catalysis, 2018, 357, 213-222.	3.1	53
40	Near-infrared absorption of Ï€-stacking columns composed of trioxotriangulene neutral radicals. Npj Quantum Materials, 2017, 2, .	1.8	52
41	Local unitary transformation method for large-scale two-component relativistic calculations. II. Extension to two-electron Coulomb interaction. Journal of Chemical Physics, 2012, 137, 144101.	1.2	51
42	Theoretical study on molecular and dissociative chemisorptions of an O2 molecule on an Ag surface: dipped adcluster model combined with symmetry-adapted cluster-configuration interaction method. Chemical Physics Letters, 1990, 174, 283-286.	1.2	49
43	Ï€*â€“Ïƒ* hyperconjugation mechanism on the rotational barrier of the methyl group (I): Substituted toluenes in the ground, excited, and anionic states. Journal of Chemical Physics, 2000, 113, 2168-2174.	1.2	48
44	Extension of the Core-Valence-Rydberg B3LYP Functional to Core-Excited-State Calculations of Third-Row Atoms. Journal of Chemical Theory and Computation, 2007, 3, 1295-1305.	2.3	46
45	Reconsidering an analytical gradient expression within a divide-and-conquer self-consistent field approach: Exact formula and its approximate treatment. Journal of Chemical Physics, 2011, 134, 034105.	1.2	45
46	Dipped adcluster model for chemisorptions and catalytic reactions on a metal surface: Image force correction and applications to Pdâ€“O2 adclusters. Journal of Chemical Physics, 1991, 95, 640-647.	1.2	43
47	Oxidation mechanism of propylene on an Ag surface: dipped adcluster model study. Surface Science, 1998, 401, 371-391.	0.8	43
48	Description of core excitations by time-dependent density functional theory with local density approximation, generalized gradient approximation, meta-generalized gradient approximation, and hybrid functionals. Journal of Computational Chemistry, 2007, 28, 2067-2074.	1.5	43
49	Analysis of self-interaction correction for describing core excited states. International Journal of Quantum Chemistry, 2007, 107, 23-29.	1.0	43
50	Divide-and-conquer self-consistent field calculation for open-shell systems: Implementation and application. Chemical Physics Letters, 2010, 500, 172-177.	1.2	43
51	Ab Initio Molecular Orbital Study on the Oxidation Mechanism for Dimethylamine Borane as a Reductant for an Electroless Deposition Process. Journal of Physical Chemistry B, 1999, 103, 1774-1778.	1.2	42
52	Is the divide-and-conquer Hartreeâ€“Fock method valid for calculations of delocalized systems?. Molecular Physics, 2007, 105, 2799-2804.	0.8	42
53	Ab Initio Molecular Orbital Study of the Oxidation Mechanism of Hypophosphite Ion as a Reductant for an Electroless Deposition Process. Journal of Physical Chemistry B, 2001, 105, 1701-1704.	1.2	41
54	Reactions of protonated water clusters H+(H2O)n (n=1â€“6) with dimethylsulfoxide in a guided ion beam apparatus. Chemical Physics Letters, 2003, 377, 69-73.	1.2	41

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55	Rigorous non-Born-Oppenheimer theory: Combination of explicitly correlated Gaussian method and nuclear orbital plus molecular orbital theory. Journal of Chemical Physics, 2011, 135, 024111.	1.2	41
56	Theoretical study on the photostimulated desorption of CO from a Pt surface. Journal of Chemical Physics, 1996, 104, 714-726.	1.2	38
57	Nature of the change in the rotational barrier of the methyl group due to S0â†'S1 excitation. Chemical Physics Letters, 1999, 307, 272-276.	1.2	38
58	Divide-and-Conquer-Type Density-Functional Tight-Binding Simulations of Hydroxide Ion Diffusion in Bulk Water. Journal of Physical Chemistry B, 2017, 121, 1362-1371.	1.2	38
59	Rigorous pK_a Estimation of Amine Species Using Density-Functional Tight-Binding-Based Metadynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 351-356.	2.3	38
60	Implementation of SurjÃ¡nâ€™s density matrix formulae for calculating second-order MÃ¸llerâ€“Plesset energy. Chemical Physics Letters, 2006, 420, 250-255.	1.2	37
61	Elimination of translational and rotational motions in nuclear orbital plus molecular orbital theory: Application of MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2006, 124, 194110.	1.2	37
62	Potential energy curves of dioxygen anion species, Oâ^'2 and O2â^'2. Chemical Physics Letters, 1992, 197, 339-345.	1.2	36
63	EXTENSION OF ENERGY DENSITY ANALYSIS TO TREATING CHEMICAL BONDS IN MOLECULES. Journal of Theoretical and Computational Chemistry, 2005, 04, 317-331.	1.8	36
64	Colleâ€“Salvettiâ€type correction for electronâ€“nucleus correlation in the nuclear orbital plus molecular orbital theory. Journal of Computational Chemistry, 2008, 29, 735-740.	1.5	36
65	Novel Approach to Excited-State Calculations of Large Molecules Based on Divide-and-Conquer Method: Application to Photoactive Yellow Protein. Journal of Physical Chemistry B, 2013, 117, 5565-5573.	1.2	36
66	Revisiting the extrapolation of correlation energies to complete basis set limit. Journal of Computational Chemistry, 2015, 36, 1075-1082.	1.5	36
67	Time-dependent Hartreeâ€“Fock frequency-dependent polarizability calculation applied to divide-and-conquer electronic structure method. Chemical Physics Letters, 2010, 485, 247-252.	1.2	35
68	Quantum chemistry beyond Bornâ€“Oppenheimer approximation on a quantum computer: A simulated phase estimation study. International Journal of Quantum Chemistry, 2016, 116, 1328-1336.	1.0	35
69	Dipped adcluster model study for the end-on chemisorption of O2 on an Ag surface. Canadian Journal of Chemistry, 1992, 70, 404-408.	0.6	34
70	Mechanism of the partial oxidation of ethylene on an Ag surface: dipped adcluster model study. Surface Science, 1997, 384, 315-333.	0.8	34
71	Grid-based energy density analysis: Implementation and assessment. Journal of Chemical Physics, 2007, 126, 034103.	1.2	34
72	Short-time Fourier transform analysis of real-time time-dependent Hartreeâ€“Fock and time-dependent density functional theory calculations with Gaussian basis functions. Journal of Chemical Physics, 2010, 132, 054104.	1.2	34

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73	Linearity condition for orbital energies in density functional theory: Construction of orbital-specific hybrid functional. Journal of Chemical Physics, 2011, 134, 124113.	1.2	34
74	Contrasting mechanisms for CO2 absorption and regeneration processes in aqueous amine solutions: Insights from density-functional tight-binding molecular dynamics simulations. Chemical Physics Letters, 2016, 647, 127-131.	1.2	34
75	Orbital-free density functional theory calculation applying semi-local machine-learned kinetic energy density functional and kinetic potential. Chemical Physics Letters, 2020, 748, 137358.	1.2	34
76	Density Functional Theory Analysis of Reaction Mechanism of Hypophosphite Ions on Metal Surfaces. Journal of the Electrochemical Society, 2011, 158, D585.	1.3	33
77	DFT Calculation Analysis of the Infrared Spectra of Ethylene Adsorbed on Cu(110), Pd(110), and Ag(110). Journal of Physical Chemistry B, 2002, 106, 10714-10721.	1.2	32
78	Synthesis of the Pivalamidate-Bridged Pentanuclear Platinum(II,III) Linear Complexes with PtÂ·Â·Â·Pt Interactions. Inorganic Chemistry, 2005, 44, 8552-8560.	1.9	32
79	Time-dependent density functional theory (TDDFT) calculations for core-excited states: Assessment of an exchange functional combining the Becke88 and van Leeuwenâ€“Baerends-type functionals. Chemical Physics Letters, 2006, 419, 297-303.	1.2	32
80	Divide-and-Conquer Density-Functional Tight-Binding Molecular Dynamics Study on the Formation of Carbamate Ions during CO2 Chemical Absorption in Aqueous Amine Solution. Bulletin of the Chemical Society of Japan, 2017, 90, 1230-1235.	2.0	32
81	Semi-local machine-learned kinetic energy density functional demonstrating smooth potential energy curves. Chemical Physics Letters, 2019, 734, 136732.	1.2	32
82	A hybrid approach combining energy density analysis with the interaction energy decomposition method. Journal of Computational Chemistry, 2004, 25, 1882-1887.	1.5	31
83	Extension of energy density analysis to periodic boundary condition calculation: Evaluation of locality in extended systems. Chemical Physics Letters, 2007, 438, 132-138.	1.2	31
84	Electronic temperature in divideâ€andâ€conquer electronic structure calculation revisited: Assessment and improvement of selfâ€consistent field convergence. International Journal of Quantum Chemistry, 2009, 109, 2706-2713.	1.0	31
85	Theoretical study on the ground and excited states of the chromate anion CrO2â¯4. Journal of Chemical Physics, 1994, 101, 1029-1036.	1.2	29
86	CO and NO adsorption on copper-containing zeolite. A theoretical ab initio study. Catalysis Letters, 1996, 42, 173-176.	1.4	29
87	Energy density analysis of cluster size dependence of surface-molecule interactions: H2, C2H2, C2H4, and CO adsorption onto Si(100)-(2Ã—1) surface. Journal of Chemical Physics, 2004, 121, 4893-4900.	1.2	29
88	Cristaxenicin A, an Antiprotozoal Xenicane Diterpenoid from the Deep Sea Gorgonian Acanthoprimnoa cristata. Journal of Organic Chemistry, 2012, 77, 10962-10966.	1.7	29
89	Local unitary transformation method toward practical electron correlation calculations with scalar relativistic effect in large-scale molecules. Journal of Chemical Physics, 2013, 139, 034109.	1.2	29
90	Parallel implementation of efficient chargeâ€“charge interaction evaluation scheme in periodic divideâ€andâ€conquer densityâ€functional tightâ€binding calculations. Journal of Computational Chemistry, 2018, 39, 105-116.	1.5	29

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91	The important role of N2H formation energy for low-temperature ammonia synthesis in an electric field. Catalysis Today, 2020, 351, 119-124.	2.2	29
92	Electronic mechanism of the surface enhanced Raman scattering. Journal of Chemical Physics, 1995, 103, 2286-2294.	1.2	28
93	Linearity condition for orbital energies in density functional theory (II): Application to global hybrid functionals. Chemical Physics Letters, 2011, 513, 130-135.	1.2	28
94	Simulations of the synthesis of boron-nitride nanostructures in a hot, high pressure gas volume. Chemical Science, 2018, 9, 3803-3819.	3.7	28
95	Energy density analysis (EDA) of cis, trans-enol isomerization in malonaldehyde, tropolone and 9-hydroxyphenalenone. Chemical Physics Letters, 2002, 365, 203-210.	1.2	27
96	Density Functional Theory Analysis for Orbital Interaction between Hypophosphite Ions and Metal Surfaces. Journal of the Electrochemical Society, 2011, 158, D626.	1.3	27
97	Divide-and-Conquer Approaches to Quantum Chemistry: Theory and Implementation. Challenges and Advances in Computational Chemistry and Physics, 2011, , 97-127.	0.6	27
98	Hybrid approach for ab initio molecular dynamics simulation combining energy density analysis and short-time Fourier transform: Energy transfer spectrogram. Journal of Chemical Physics, 2005, 123, 034101.	1.2	26
99	Interpretation of Intermolecular Geometric Isotope Effect in Hydrogen Bonds: Nuclear Orbital plus Molecular Orbital Study. Journal of Physical Chemistry A, 2011, 115, 1433-1439.	1.1	26
100	Linear-scaling divide-and-conquer second-order MÃ¸llerâ€“Plesset perturbation calculation for open-shell systems: implementation and application. Theoretical Chemistry Accounts, 2011, 130, 411-417.	0.5	26
101	Electron-Hopping Brings Lattice Strain and High Catalytic Activity in the Low-Temperature Oxidative Coupling of Methane in an Electric Field. Journal of Physical Chemistry C, 2018, 122, 2089-2096.	1.5	26
102	Ï€*â€“Ïƒ* Hyperconjugation mechanism on the rotational barrier of the methyl group (II): 1- and 2-methylnaphthalenes in the S0, S1, C0, and A1 states. Chemical Physics Letters, 2000, 318, 298-304.	1.2	25
103	Non-Bornâ€“Oppenheimer effects predicted by translation-free nuclear orbital plus molecular orbital method. Chemical Physics Letters, 2006, 421, 72-76.	1.2	25
104	Development of an excited-state calculation method for large systems using dynamical polarizability: A divide-and-conquer approach at the time-dependent density functional level. Journal of Chemical Physics, 2017, 146, 124123.	1.2	25
105	Theoretical studies on the catalytic activity of Ag surface for the oxidation of olefins. International Journal of Quantum Chemistry, 1997, 65, 839-855.	1.0	24
106	Elimination of Translational and Rotational Motions in Nuclear Orbital Plus Molecular Orbital Theory:â€‰ Contribution of the First-Order Rovibration Coupling. Journal of Chemical Theory and Computation, 2006, 2, 1544-1550.	2.3	24
107	UVâ^Visible and1H or13C NMR Spectroscopic Studies on the Specific Interaction between Lithium Ions and the Anion from Tropolone or 4-Isopropyltropolone (Hinokitiol) and on the Formation of Protonated Tropolones in Acetonitrile or Other Solvents. Journal of Physical Chemistry B, 2007, 111, 1759-1768.	1.2	24
108	Quantum chemical approach for condensed-phase thermochemistry (III): Accurate evaluation of proton hydration energy and standard hydrogen electrode potential. Chemical Physics Letters, 2016, 650, 159-164.	1.2	24

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109	Theoretical investigation on structural effects of Ptâ€“Mn catalyst on activity and selectivity for methylcyclohexane dehydrogenation. Chemical Physics Letters, 2018, 711, 73-76.	1.2	24
110	Machine-learned electron correlation model based on correlation energy density at complete basis set limit. Journal of Chemical Physics, 2019, 151, 024104.	1.2	24
111	GPUâ€Accelerated Largeâ€Scale Excitedâ€State Simulation Based on Divideâ€andâ€Conquer Timeâ€Dependent Densityâ€Functional Tightâ€Binding. Journal of Computational Chemistry, 2019, 40, 2778-2786.	1.5	24
112	Natural atomic orbital based energy density analysis: Implementation and applications. Chemical Physics Letters, 2006, 424, 193-198.	1.2	23
113	Linearâ€scaling selfâ€consistent field calculations based on divideâ€andâ€conquer method using resolutionâ€ofâ€identity approximation on graphical processing units. Journal of Computational Chemistry, 2015, 36, 164-170.	1.5	23
114	Quantum mechanical molecular dynamics simulations of polaron formation in methylammonium lead iodide perovskite. Physical Chemistry Chemical Physics, 2020, 22, 97-106.	1.3	23
115	Energy density analysis of internal methyl rotations in halogenated toluenes. Chemical Physics Letters, 2003, 368, 673-679.	1.2	22
116	Energy density analysis (EDA) of proton transfer reactions in malonaldehyde, tropolone, and 9-hydroxyphenalenone. Computational and Theoretical Chemistry, 2003, 637, 27-35.	1.5	22
117	Extension of Density Functional Theory to Nuclear Orbital plus Molecular Orbital Theory: Self-Consistent Field Calculations with the Colleâ€“Salvetti Electronâ€“Nucleus Correlation Functional. Bulletin of the Chemical Society of Japan, 2009, 82, 1133-1139.	2.0	22
118	Accelerating convergence in the antisymmetric product of strongly orthogonal geminals method. International Journal of Quantum Chemistry, 2013, 113, 239-244.	1.0	22
119	An effective energy gradient expression for divide-and-conquer second-order MÃ¸llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2013, 138, 044102.	1.2	22
120	Large-Scale Molecular Dynamics Simulation for Ground and Excited States Based on Divide-and-Conquer Long-Range Corrected Density-Functional Tight-Binding Method. Journal of Chemical Theory and Computation, 2020, 16, 2369-2378.	2.3	22
121	Periodic-Boundary-Condition Calculation using Heyd-Scuseria-Ernzerhof Screened Coulomb Hybrid Functional: Electronic Structure of Anatase and Rutile TiO2. Journal of Computer Chemistry Japan, 2006, 5, 7-18.	0.0	22
122	Density functional theory study on the oxidation mechanisms of aldehydes as reductants for electroless Cu deposition process. Electrochimica Acta, 2005, 51, 906-915.	2.6	21
123	Application of the Sakuraiâ€Sugiura projection method to coreâ€excitedâ€state calculation by timeâ€dependent density functional theory. Journal of Computational Chemistry, 2008, 29, 2311-2316.	1.5	21
124	Twoâ€level hierarchical parallelization of secondâ€order MÃ¸llerâ€“plesset perturbation calculations in divideâ€andâ€conquer method. Journal of Computational Chemistry, 2011, 32, 2756-2764.	1.5	21
125	Extension of local response dispersion method to excited-state calculation based on time-dependent density functional theory. Journal of Chemical Physics, 2012, 137, 124106.	1.2	21
126	Divideâ€andâ€conquerâ€based symmetry adapted cluster method: Synergistic effect of subsystem fragmentation and configuration selection. International Journal of Quantum Chemistry, 2013, 113, 218-223.	1.0	21

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127	Analytical energy gradient based on spin-free infinite-order Douglas-Kroll-Hess method with local unitary transformation. Journal of Chemical Physics, 2013, 139, 244107.	1.2	21
128	Effect of Hartree-Fock exact exchange on intramolecular magnetic coupling constants of organic diradicals. Journal of Chemical Physics, 2015, 142, 024318.	1.2	21
129	Density Functional Theory Analysis of Elementary Reactions in NO_x Reduction on Rh Surfaces and Rh Clusters. Journal of Physical Chemistry C, 2017, 121, 15272-15281.	1.5	21
130	Agglomeration Suppression of a Fe-Supported Catalyst and its Utilization for Low-Temperature Ammonia Synthesis in an Electric Field. ACS Omega, 2020, 5, 6846-6851.	1.6	21
131	Quantum chemical approach for condensed-phase thermochemistry: Proposal of a harmonic solvation model. Journal of Chemical Physics, 2014, 141, 174106.	1.2	20
132	Theoretical Study on the Photochemical Decomposition Reaction of Permanganate Ion, MnO4-. The Journal of Physical Chemistry, 1995, 99, 8550-8555.	2.9	19
133	Molecular Orbital Study on the Oxidation Mechanism of Hydrazine and Hydroxylamine as Reducing Agents for Electroless Deposition Process. Electrochemistry, 2007, 75, 45-49.	0.6	19
134	Application of Real-time Time-dependent Density Functional Theory with the CVB3LYP Functional to Core Excitations. Chemistry Letters, 2010, 39, 407-409.	0.7	19
135	Theoretical Study of Extremely Long yet Stable Carbonâ€“Carbon Bonds: Effect of Attractive CÂ·Â·Â·H Interactions and Small Radical Stabilization of Diamondoids. Bulletin of the Chemical Society of Japan, 2015, 88, 1636-1641.	2.0	19
136	Electronic Structures of MoF6 and MoOF4 in the Ground and Excited States: A SAC-CI and Frozen-Orbital-Analysis Study. Journal of Physical Chemistry A, 1998, 102, 2033-2043.	1.1	18
137	Molecular orbital propagation to accelerate self-consistent-field convergence in an ab initio molecular dynamics simulation. Journal of Chemical Physics, 2008, 128, 094101.	1.2	18
138	Development of the explicitly correlated Gaussianâ€“nuclear orbital plus molecular orbital theory: Incorporation of electronâ€“electron correlation. Chemical Physics Letters, 2012, 533, 100-105.	1.2	18
139	RAQET: Largeâ€scale twoâ€component relativistic quantum chemistry program package. Journal of Computational Chemistry, 2018, 39, 2333-2344.	1.5	18
140	Sodiumâ€and Potassiumâ€Hydrate Melts Containing Asymmetric Imide Anions for Highâ€Voltage Aqueous Batteries. Angewandte Chemie, 2019, 131, 14340-14345.	1.6	18
141	An Airâ€and Waterâ€Stable B₄N₄â€Heteropentalene Serving as a Host Material for a Phosphorescent OLED. Angewandte Chemie - International Edition, 2021, 60, 23812-23818.	7.2	18
142	Theoretical study on ammonia cluster ions: nature of thermodynamic magic number. Chemical Physics, 2000, 262, 201-210.	0.9	17
143	Size-Dependent Reaction Cross Section of Protonated Water Clusters H+(H2O)n(n= 2â^'11) with D2O. Journal of Physical Chemistry A, 2003, 107, 10904-10910.	1.1	17
144	Isotope effect in dihydrogen-bonded systems: application of the analytical energy gradient method in the nuclear orbital plus molecular orbital theory. Molecular Physics, 2007, 105, 2649-2657.	0.8	17

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145	Dynamic hyperpolarizability calculations of large systems: The linear-scaling divide-and-conquer approach. Journal of Chemical Physics, 2012, 136, 084108.	1.2	17
146	Selfâ€consistent field treatment and analytical energy gradient of local response dispersion method. International Journal of Quantum Chemistry, 2013, 113, 257-262.	1.0	17
147	Density-Functional Tight-Binding Molecular Dynamics Simulations of Excess Proton Diffusion in Ice I_h, Ice I_c, Ice III, and Melted Ice VI Phases. Journal of Physical Chemistry A, 2018, 122, 33-40.	1.1	17
148	Development of Large-Scale Excited-State Calculations Based on the Divide-and-Conquer Time-Dependent Density Functional Tight-Binding Method. Journal of Chemical Theory and Computation, 2019, 15, 1719-1727.	2.3	17
149	Quantum Chemical Reaction Prediction Method Based on Machine Learning. Bulletin of the Chemical Society of Japan, 2020, 93, 685-693.	2.0	17
150	Energy density analysis of embedded cluster models for an MgO crystal. Chemical Physics Letters, 2005, 410, 64-69.	1.2	16
151	Energy density analysis of cluster size dependence of surface-molecule interactions (II): Formate adsorption onto a Cu(111) surface. Journal of Computational Chemistry, 2006, 27, 917-925.	1.5	16
152	Improving quasiparticle second order electron propagator calculations with the spin-component-scaled technique. Chemical Physics Letters, 2014, 591, 82-87.	1.2	16
153	Hydroxide Ion Carrier for Proton Pumps in Bacteriorhodopsin: Primary Proton Transfer. Journal of Physical Chemistry B, 2020, 124, 8524-8539.	1.2	16
154	Simulating the Coupled Structuralâ€“Electronic Dynamics of Photoexcited Lead Iodide Perovskites. Journal of Physical Chemistry Letters, 2020, 11, 4448-4455.	2.1	16
155	Implementation of Divide-and-Conquer (DC) Electronic Structure Code to GAMESS Program Package. Journal of Computer Chemistry Japan, 2009, 8, 1-12.	0.0	16
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