Hiromi Nakai

List of Publications by Citations

336 papers	6,956 citations	40 h-index	65 g-index
350 ext. papers	7,755 ext. citations	3.6 avg, IF	6.44 L-index

#	Paper	IF	Citations
336	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	16.4	192
335	An extension of ab initio molecular orbital theory to nuclear motion. *Chemical Physics Letters*, **1998**, 290, 437-442	2.5	192
334	Density functional method including weak interactions: Dispersion coefficients based on the local response approximation. *Journal of Chemical Physics*, **2009**, 131, 224104	3.9	188
333	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	3.9	186
332	Theoretical Analysis on De-Solvation of Lithium, Sodium, and Magnesium Cations to Organic Electrolyte Solvents. *Journal of the Electrochemical Society*, **2013**, 160, A2160-A2165	3.9	175
331	Alternative linear-scaling methodology for the second-order M□ller-Plesset perturbation calculation based on the divide-and-conquer method. *Journal of Chemical Physics*, **2007**, 127, 074103	3.9	129
330	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	3.9	124
329	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	3.9	118
328	Energy density analysis with Kohn□Sham orbitals. *Chemical Physics Letters*, **2002**, 363, 73-79	2.5	116
327	Implementation of divide-and-conquer method including Hartree-Fock exchange interaction. *Journal of Computational Chemistry*, **2007**, 28, 2003-12	3.5	114
326	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	2.1	107
325	Many-body effects in nonadiabatic molecular theory for simultaneous determination of nuclear and electronic wave functions: Ab initio NOMO/MBPT and CC methods. *Journal of Chemical Physics*, **2003**, 118, 1119-1127	3.9	89
324	Local response dispersion method. II. Generalized multicenter interactions. *Journal of Chemical Physics*, **2010**, 133, 194101	3.9	82
323	Nuclear orbital plus molecular orbital theory: Simultaneous determination of nuclear and electronic wave functions without Born□Oppenheimer approximation. *International Journal of Quantum Chemistry*, **2007**, 107, 2849-2869	2.1	77
322	Ab initio molecular orbital model of scanning tunneling microscopy. *Journal of Chemical Physics*, **1996**, 104, 2410-2417	3.9	74
321	Three pillars for achieving quantum mechanical molecular dynamics simulations of huge systems: Divide-and-conquer, density-functional tight-binding, and massively parallel computation. *Journal of Computational Chemistry*, **2016**, 37, 1983-92	3.5	72
320	Dipped adcluster model study for molecular and dissociative chemisorptions of O2 on Ag surface. *Journal of Chemical Physics*, **1993**, 98, 2423-2436	3.9	67

319	Second-order Møller-Plesset perturbation energy obtained from divide-and-conquer Hartree-Fock density matrix. *Journal of Chemical Physics*, **2006**, 125, 204106	3.9	64
318	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, 7629-39	3.6	63
317	Molecular orbital study on the reaction process of dimethylamine borane as a reductant for electroless deposition. *Journal of Electroanalytical Chemistry*, **2003**, 559, 131-136	4.1	63
316	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, 94105	3.9	62
315	Confined water-mediated high proton conduction in hydrophobic channel of a synthetic nanotube. *Nature Communications*, **2020**, 11, 843	17.4	61
314	Non-Born□Oppenheimer theory for simultaneous determination of vibrational and electronic excited states: ab initio NO+MO/CIS theory. *Chemical Physics Letters*, **2001**, 345, 118-124	2.5	60
313	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	3.9	59
312	Activation of O2 on Cu, Ag, and Au surfaces for the epoxidation of ethylene: dipped adcluster model study. *Surface Science*, **1997**, 387, 328-341	1.8	58
311	Dual-level hierarchical scheme for linear-scaling divide-and-conquer correlation theory. *International Journal of Quantum Chemistry*, **2009**, 109, 2227-2237	2.1	57
310	Elimination of translational and rotational motions in nuclear orbital plus molecular orbital theory. *Journal of Chemical Physics*, **2005**, 122, 164101	3.9	57
309	Molecular orbital study on the reaction mechanisms of electroless deposition processes. *Electrochimica Acta*, **2001**, 47, 47-53	6.7	57
308	Hybrid exchange-correlation functional for core, valence, and Rydberg excitations: core-valence-Rydberg B3LYP. *Journal of Chemical Physics*, **2006**, 125, 64109	3.9	56
307	Theoretical study on the ground and excited states of MnO_4^{2-}. *Journal of Chemical Physics*, **1991**, 95, 8287-8291	3.9	53
306	Sodium- and Potassium-Hydrate Melts Containing Asymmetric Imide Anions for High-Voltage Aqueous Batteries. *Angewandte Chemie - International Edition*, **2019**, 58, 14202-14207	16.4	51
305	Assessment of self-consistent field convergence in spin-dependent relativistic calculations. *Chemical Physics Letters*, **2016**, 657, 65-71	2.5	48
304	Theoretical Analysis of Carrier Ion Diffusion in Superconcentrated Electrolyte Solutions for Sodium-Ion Batteries. *Journal of Physical Chemistry B*, **2018**, 122, 2600-2609	3.4	46
303	Generalized Møller-Plesset Partitioning in Multiconfiguration Perturbation Theory. *Journal of Chemical Theory and Computation*, **2010**, 6, 2024-33	6.4	45
302	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	2.5	44

301	Semi-local machine-learned kinetic energy density functional with third-order gradients of electron density. *Journal of Chemical Physics*, **2018**, 148, 241705	3.9	43
300	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	3.9	42
299	□□ 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	3.9	42
298	Reversible Sodium Metal Electrodes: Is Fluorine an Essential Interphasial Component?. *Angewandte Chemie - International Edition*, **2019**, 58, 8024-8028	16.4	41
297	Near-infrared absorption of □stacking columns composed of trioxotriangulene neutral radicals. *Npj Quantum Materials*, **2017**, 2,	5	41
296	Divide-and-conquer self-consistent field calculation for open-shell systems: Implementation and application. *Chemical Physics Letters*, **2010**, 500, 172-177	2.5	40
295	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, 217-21	3.4	39
294	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	3.9	39
293	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	3.4	39
292	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	3.9	38
291	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, 1295-305	6.4	38
290	Is the divide-and-conquer Hartree□Fock method valid for calculations of delocalized systems?. *Molecular Physics*, **2007**, 105, 2799-2804	1.7	38
289	Dipped adcluster model for chemisorptions and catalytic reactions on a metal surface: Image force correction and applications to Pd□2 adclusters. *Journal of Chemical Physics*, **1991**, 95, 640-647	3.9	38
288	Catalytic performance of Ru, Os, and Rh nanoparticles for ammonia synthesis: A density functional theory analysis. *Journal of Catalysis*, **2018**, 357, 213-222	7.3	38
287	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	3.4	37
286	Oxidation mechanism of propylene on an Ag surface: dipped adcluster model study. *Surface Science* , **1998**, 401, 371-391	1.8	36
285	Analysis of self-interaction correction for describing core excited states. *International Journal of Quantum Chemistry*, **2007**, 107, 23-29	2.1	36
284	EXTENSION OF ENERGY DENSITY ANALYSIS TO TREATING CHEMICAL BONDS IN MOLECULES. *Journal of Theoretical and Computational Chemistry*, **2005**, 04, 317-331	1.8	36

283	Implementation of Surj□□ density matrix formulae for calculating second-order M□ller-Plesset energy. *Chemical Physics Letters*, **2006**, 420, 250-255	2.5	36
282	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, 2067-74	3.5	35
281	Reactions of protonated water clusters H+(H2O)n (n=1-8) with dimethylsulfoxide in a guided ion beam apparatus. *Chemical Physics Letters*, **2003**, 377, 69-73	2.5	35
280	Theoretical study on the photostimulated desorption of CO from a Pt surface. *Journal of Chemical Physics*, **1996**, 104, 714-726	3.9	35
279	Elimination of translational and rotational motions in nuclear orbital plus molecular orbital theory: application of Moller-Plesset perturbation theory. *Journal of Chemical Physics*, **2006**, 124, 194110	3.9	34
278	Time-dependent Hartree-Fock frequency-dependent polarizability calculation applied to divide-and-conquer electronic structure method. *Chemical Physics Letters*, **2010**, 485, 247-252	2.5	32
277	Grid-based energy density analysis: implementation and assessment. *Journal of Chemical Physics*, **2007**, 126, 034103	3.9	32
276	Colle-Salvetti-type correction for electron-nucleus correlation in the nuclear orbital plus molecular orbital theory. *Journal of Computational Chemistry*, **2008**, 29, 735-40	3.5	32
275	Nature of the change in the rotational barrier of the methyl group due to S0-S1 excitation. *Chemical Physics Letters*, **1999**, 307, 272-276	2.5	32
274	Dcdftbmd: Divide-and-Conquer Density Functional Tight-Binding Program for Huge-System Quantum Mechanical Molecular Dynamics Simulations. *Journal of Computational Chemistry*, **2019**, 40, 1538-1549	3.5	31
273	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, 5565-73	3.4	31
272	Linearity condition for orbital energies in density functional theory: construction of orbital-specific hybrid functional. *Journal of Chemical Physics*, **2011**, 134, 124113	3.9	31
271	Mechanism of the partial oxidation of ethylene on an Ag surface: dipped adcluster model study. *Surface Science*, **1997**, 384, 315-333	1.8	31
270	Time-dependent density functional theory (TDDFT) calculations for core-excited states: Assessment of an exchange functional combining the Becke88 and van Leeuwen-Baerends-type functionals. *Chemical Physics Letters*, **2006**, 419, 297-303	2.5	31
269	A hybrid approach combining energy density analysis with the interaction energy decomposition method. *Journal of Computational Chemistry*, **2004**, 25, 1882-7	3.5	31
268	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	3.4	30
267	Extension of energy density analysis to periodic boundary condition calculation: Evaluation of locality in extended systems. *Chemical Physics Letters*, **2007**, 438, 132-138	2.5	30
266	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	3.4	30

265	Potential energy curves of dioxygen anion species, O2 and O22. *Chemical Physics Letters*, **1992**, 197, 339-345	2.5	30
264	Dipped adcluster model study for the end-on chemisorption of O2 on an Ag surface. *Canadian Journal of Chemistry*, **1992**, 70, 404-408	0.9	29
263	Rigorous pK Estimation of Amine Species Using Density-Functional Tight-Binding-Based Metadynamics Simulations. *Journal of Chemical Theory and Computation*, **2018**, 14, 351-356	6.4	29
262	Divide-and-Conquer Density-Functional Tight-Binding Molecular Dynamics Study on the Formation of Carbamate Ions during CO2Chemical Absorption in Aqueous Amine Solution. *Bulletin of the Chemical Society of Japan*, **2017**, 90, 1230-1235	5.1	28
261	Revisiting the extrapolation of correlation energies to complete basis set limit. *Journal of Computational Chemistry*, **2015**, 36, 1075-82	3.5	28
260	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	2.5	28
259	Short-time Fourier transform analysis of real-time time-dependent Hartree-Fock and time-dependent density functional theory calculations with Gaussian basis functions. *Journal of Chemical Physics*, **2010**, 132, 054104	3.9	28
258	Electronic temperature in divide-and-conquer electronic structure calculation revisited: Assessment and improvement of self-consistent field convergence. *International Journal of Quantum Chemistry*, **2009**, 109, 2706-2713	2.1	27
257	Density Functional Theory Analysis of Reaction Mechanism of Hypophosphite Ions on Metal Surfaces. *Journal of the Electrochemical Society*, **2011**, 158, D585	3.9	27
256	Synthesis of the pivalamidate-bridged pentanuclear platinum(II,III) linear complexes with Pt...Pt interactions. *Inorganic Chemistry*, **2005**, 44, 8552-60	5.1	27
255	Energy density analysis of cluster size dependence of surface-molecule interactions: H2, C2H2, C2H4, and CO adsorption onto Si(100)-(2x1) surface. *Journal of Chemical Physics*, **2004**, 121, 4893-900	3.9	27
254	Energy density analysis (EDA) of cis, trans-enol isomerization in malonaldehyde, tropolone and 9-hydroxyphenalenone. *Chemical Physics Letters*, **2002**, 365, 203-210	2.5	27
253	CO and NO adsorption on copper-containing zeolite. A theoretical ab initio study. *Catalysis Letters*, **1996**, 42, 173-176	2.8	27
252	Linearity condition for orbital energies in density functional theory (II): Application to global hybrid functionals. *Chemical Physics Letters*, **2011**, 513, 130-135	2.5	26
251	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, 34101	3.9	26
250	Electronic mechanism of the surface enhanced Raman scattering. *Journal of Chemical Physics*, **1995**, 103, 2286-2294	3.9	26
249	Non-BornOppenheimer effects predicted by translation-free nuclear orbital plus molecular orbital method. *Chemical Physics Letters*, **2006**, 421, 72-76	2.5	25
248	Divide-and-Conquer Approaches to Quantum Chemistry: Theory and Implementation. *Challenges and Advances in Computational Chemistry and Physics*, **2011**, 97-127	0.7	25

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246	Interpretation of intermolecular geometric isotope effect in hydrogen bonds: nuclear orbital plus molecular orbital study. *Journal of Physical Chemistry A*, **2011**, 115, 1433-9	2.8	24
245	Theoretical studies on the catalytic activity of Ag surface for the oxidation of olefins. *International Journal of Quantum Chemistry*, **1997**, 65, 839-855	2.1	24
244	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	2.5	24
243	Theoretical study on the ground and excited states of the chromate anion CrO_2^{2-}. *Journal of Chemical Physics*, **1994**, 101, 1029-1036	3.9	24
242	Simulations of the synthesis of boron-nitride nanostructures in a hot, high pressure gas volume. *Chemical Science*, **2018**, 9, 3803-3819	9.4	23
241	Local unitary transformation method toward practical electron correlation calculations with scalar relativistic effect in large-scale molecules. *Journal of Chemical Physics*, **2013**, 139, 034109	3.9	23
240	Linear-scaling divide-and-conquer second-order Møller–Plesset perturbation calculation for open-shell systems: implementation and application. *Theoretical Chemistry Accounts*, **2011**, 130, 411-417	1.9	23
239	Parallel implementation of efficient charge-charge interaction evaluation scheme in periodic divide-and-conquer density-functional tight-binding calculations. *Journal of Computational Chemistry*, **2018**, 39, 105-116	3.5	22
238	UV-visible and 1H or 13C 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, 1759-68	3.4	22
237	Energy density analysis of internal methyl rotations in halogenated toluenes. *Chemical Physics Letters*, **2003**, 368, 673-679	2.5	22
236	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	0.2	22
235	Linear-scaling self-consistent field calculations based on divide-and-conquer method using resolution-of-identity approximation on graphical processing units. *Journal of Computational Chemistry*, **2015**, 36, 164-70	3.5	21
234	Semi-local machine-learned kinetic energy density functional demonstrating smooth potential energy curves. *Chemical Physics Letters*, **2019**, 734, 136732	2.5	21
233	Density Functional Theory Analysis for Orbital Interaction between Hypophosphite Ions and Metal Surfaces. *Journal of the Electrochemical Society*, **2011**, 158, D626	3.9	21
232	Elimination of Translational and Rotational Motions in Nuclear Orbital Plus Molecular Orbital Theory: Contribution of the First-Order Rovibration Coupling. *Journal of Chemical Theory and Computation*, **2006**, 2, 1544-50	6.4	21
231	Natural atomic orbital based energy density analysis: Implementation and applications. *Chemical Physics Letters*, **2006**, 424, 193-198	2.5	21
230	Energy density analysis (EDA) of proton transfer reactions in malonaldehyde, tropolone, and 9-hydroxyphenalenone. *Computational and Theoretical Chemistry*, **2003**, 637, 27-35		21

229	Density functional theory study on the oxidation mechanisms of aldehydes as reductants for electroless Cu deposition process. *Electrochimica Acta*, **2005**, 51, 906-915	6.7	21
228	Quantum chemistry beyond Born□Oppenheimer approximation on a quantum computer: A simulated phase estimation study. *International Journal of Quantum Chemistry*, **2016**, 116, 1328-1336	2.1	21
227	Accelerating convergence in the antisymmetric product of strongly orthogonal geminals method. *International Journal of Quantum Chemistry*, **2013**, 113, 239-244	2.1	19
226	An effective energy gradient expression for divide-and-conquer second-order M□ller-Plesset perturbation theory. *Journal of Chemical Physics*, **2013**, 138, 044102	3.9	19
225	Extension of Density Functional Theory to Nuclear Orbital plus Molecular Orbital Theory: Self-Consistent Field Calculations with the Colle□Salvetti Electron□Nucleus Correlation Functional. *Bulletin of the Chemical Society of Japan*, **2009**, 82, 1133-1139	5.1	19
224	Application of the Sakurai-Sugiura projection method to core-excited-state calculation by time-dependent density functional theory. *Journal of Computational Chemistry*, **2008**, 29, 2311-6	3.5	19
223	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	3.9	18
222	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	3.8	18
221	Divide-and-conquer-based symmetry adapted cluster method: Synergistic effect of subsystem fragmentation and configuration selection. *International Journal of Quantum Chemistry*, **2013**, 113, 218-223	2.1	18
220	Quantum chemical approach for condensed-phase thermochemistry: proposal of a harmonic solvation model. *Journal of Chemical Physics*, **2014**, 141, 174106	3.9	18
219	Two-level hierarchical parallelization of second-order M□ller-Plesset perturbation calculations in divide-and-conquer method. *Journal of Computational Chemistry*, **2011**, 32, 2756-64	3.5	18
218	Machine-learned electron correlation model based on correlation energy density at complete basis set limit. *Journal of Chemical Physics*, **2019**, 151, 024104	3.9	17
217	Density Functional Theory Analysis of Elementary Reactions in NOx Reduction on Rh Surfaces and Rh Clusters. *Journal of Physical Chemistry C*, **2017**, 121, 15272-15281	3.8	17
216	Effect of Hartree-Fock exact exchange on intramolecular magnetic coupling constants of organic diradicals. *Journal of Chemical Physics*, **2015**, 142, 024318	3.9	17
215	Molecular orbital propagation to accelerate self-consistent-field convergence in an ab initio molecular dynamics simulation. *Journal of Chemical Physics*, **2008**, 128, 094101	3.9	17
214	Theoretical study on ammonia cluster ions: nature of thermodynamic magic number. *Chemical Physics*, **2000**, 262, 201-210	2.3	17
213	Theoretical Study on the Photochemical Decomposition Reaction of Permanganate Ion, MnO4-. *The Journal of Physical Chemistry*, **1995**, 99, 8550-8555		17
212	Theoretical investigation on structural effects of Pt□Mn catalyst on activity and selectivity for methylcyclohexane dehydrogenation. *Chemical Physics Letters*, **2018**, 711, 73-76	2.5	17

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210	Self-consistent field treatment and analytical energy gradient of local response dispersion method. *International Journal of Quantum Chemistry*, **2013**, 113, 257-262	2.1	16
209	Analytical energy gradient based on spin-free infinite-order Douglas-Kroll-Hess method with local unitary transformation. *Journal of Chemical Physics*, **2013**, 139, 244107	3.9	16
208	Extension of local response dispersion method to excited-state calculation based on time-dependent density functional theory. *Journal of Chemical Physics*, **2012**, 137, 124106	3.9	16
207	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, 917-25	3.5	16
206	Molecular Orbital Study on the Oxidation Mechanism of Hydrazine and Hydroxylamine as Reducing Agents for Electroless Deposition Process. *Electrochemistry*, **2007**, 75, 45-49	1.2	16
205	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	1.7	16
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203	Energy density analysis of embedded cluster models for an MgO crystal. *Chemical Physics Letters*, **2005**, 410, 64-69	2.5	16
202	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	6.4	15
201	Development of the explicitly correlated Gaussian−nuclear orbital plus molecular orbital theory: Incorporation of electron−electron correlation. *Chemical Physics Letters*, **2012**, 533, 100-105	2.5	15
200	Dynamic hyperpolarizability calculations of large systems: the linear-scaling divide-and-conquer approach. *Journal of Chemical Physics*, **2012**, 136, 084108	3.9	15
199	Application of Real-time Time-dependent Density Functional Theory with the CVB3LYP Functional to Core Excitations. *Chemistry Letters*, **2010**, 39, 407-409	1.7	15
198	Implementation of Divide-and-Conquer (DC) Electronic Structure Code to GAMESS Program Package. *Journal of Computer Chemistry Japan*, **2009**, 8, 1-12	0.2	15
197	The important role of N2H formation energy for low-temperature ammonia synthesis in an electric field. *Catalysis Today*, **2020**, 351, 119-124	5.3	15
196	Orbital-free density functional theory calculation applying semi-local machine-learned kinetic energy density functional and kinetic potential. *Chemical Physics Letters*, **2020**, 748, 137358	2.5	14
195	Direct alkoxysilylation of alkoxysilanes for the synthesis of explicit alkoxysiloxane oligomers. *Journal of Organometallic Chemistry*, **2012**, 716, 26-31	2.3	14
194	UV−visible, 1H and 13C NMR spectroscopic studies on the interaction between protons or alkaline earth metal ions and the benzoate ion in acetonitrile. *Journal of Molecular Liquids*, **2009**, 145, 152-157	6	14

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192	Discovery of hexacoordinate hypervalent carbon compounds: Density functional study. *Chemical Physics Letters*, **2008**, 460, 37-41	2.5	14
191	Short-time Fourier transform analysis of ab initio molecular dynamics simulation: collision reaction between NH+4 (NH3)2 and NH3. *Journal of Chemical Physics*, **2004**, 121, 11098-103	3.9	14
190	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	2.8	14
189	GPU-Accelerated Large-Scale Excited-State Simulation Based on Divide-and-Conquer Time-Dependent Density-Functional Tight-Binding. *Journal of Computational Chemistry*, **2019**, 40, 2778-2786	3.5	13
188	Theoretical Study of Extremely Long yet Stable Carbon–Carbon Bonds: Effect of Attractive C–H Interactions and Small Radical Stabilization of Diamondoids. *Bulletin of the Chemical Society of Japan*, **2015**, 88, 1636-1641	5.1	13
187	Acceleration of self-consistent-field convergence in ab initio molecular dynamics and Monte Carlo simulations and geometry optimization. *Chemical Physics Letters*, **2010**, 490, 102-108	2.5	13
186	Hybrid treatment combining the translation- and rotation-free nuclear orbital plus molecular orbital theory with generator coordinate method: TRF-NOMO/GCM. *Chemical Physics Letters*, **2007**, 433, 409-415	2.5	13
185	Energy density analysis for second-order Møller-Plesset perturbation theory and coupled-cluster theory with singles and doubles: application to C2H4--CH4 complexes. *Journal of Computational Chemistry*, **2008**, 29, 1555-63	3.5	13
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