Hiromi Nakai

List of Publications by Year in Descending Order

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	Multiscale Simulation of Irregular Shape Evolution during the Initial Stage of Zn Electrodeposition on a Negative Electrode Surface. *Journal of Physical Chemistry C*, **2022**, 126, 5224-5232	3.8	1
335	Multiple protonation states in ligand-free SARS-CoV-2 main protease revealed by large-scale quantum molecular dynamics simulations.. *Chemical Physics Letters*, **2022**, 794, 139489	2.5	2
334	Analysis of the behavior of Zn atoms with a Pb additive on the surface during Zn electrodeposition. *Electrochemistry Communications*, **2022**, 138, 107291	5.1	0
333	Is Oxygen Diffusion Faster in Bulk CeO2 or on a (111)-CeO2 Surface? A Theoretical Study. *Chemistry Letters*, **2021**, 50, 568-571	1.7	1
332	Development of Linear-Scaling Relativistic Quantum Chemistry Covering the Periodic Table. *Bulletin of the Chemical Society of Japan*, **2021**, 94, 1664-1681	5.1	1
331	Assessing locally range-separated hybrid functionals from a gradient expansion of the exchange energy density. *Journal of Chemical Physics*, **2021**, 154, 214101	3.9	2
330	Innentitelbild: An Element-Substituted Cyclobutadiene Exhibiting High-Energy Blue Phosphorescence (Angew. Chem. 40/2021). *Angewandte Chemie*, **2021**, 133, 21766-21766	3.6	
329	An Element-Substituted Cyclobutadiene Exhibiting High-Energy Blue Phosphorescence. *Angewandte Chemie*, **2021**, 133, 21988-21994	3.6	2
328	An Element-Substituted Cyclobutadiene Exhibiting High-Energy Blue Phosphorescence. *Angewandte Chemie - International Edition*, **2021**, 60, 21817-21823	16.4	5
327	Robust design of D-□A model compounds using digital structures for organic DSSC applications. *Journal of Molecular Graphics and Modelling*, **2021**, 102, 107798	2.8	2
326	Theoretical prediction by DFT and experimental observation of heterocation-doping effects on hydrogen adsorption and migration over the CeO(111) surface. *Physical Chemistry Chemical Physics*, **2021**, 23, 4509-4516	3.6	3
325	Effects of A-site composition of perovskite (Sr Ba ZrO) oxides on H atom adsorption, migration, and reaction.. *RSC Advances*, **2021**, 11, 7621-7626	3.7	0
324	Picture-change correction in relativistic density functional theory. *Physical Chemistry Chemical Physics*, **2021**, 23, 15458-15474	3.6	1
323	Commentary toward the 20th Anniversary of the Society ofComputer Chemistry, Japan. *Journal of Computer Chemistry Japan*, **2021**, 20, A26-A40	0.2	
322	Trajectory Surface Hopping Approach to Condensed-Phase Nonradiative Relaxation Dynamics Using Divide-and-Conquer Spin-Flip Time-Dependent Density-Functional Tight Binding. *Journal of Chemical Theory and Computation*, **2021**, 17, 1290-1300	6.4	3
321	Database-assisted local unitary transformation method for two-electron integrals in two-component relativistic calculations. *Chemical Physics Letters*, **2021**, 777, 138691	2.5	0
320	Quantum-Mechanical Molecular Dynamics Simulations on Secondary Proton Transfer in Bacteriorhodopsin Using Realistic Models. *Journal of Physical Chemistry B*, **2021**, 125, 10947-10963	3.4	2

319	An Air- and Water-Stable B4N4-Heteropentalene Serving as a Host Material for a Phosphorescent OLED. *Angewandte Chemie*, **2021**, 133, 24005	3.6	1
318	An Air- and Water-Stable B N -Heteropentalene Serving as a Host Material for a Phosphorescent OLED. *Angewandte Chemie - International Edition*, **2021**, 60, 23812-23818	16.4	3
317	Development of Quantum Algorithm qUCC-LR for Excited-State Calculation Using Dynamic Polarizability. *Journal of Computer Chemistry Japan*, **2021**, 20, 140-143	0.2	
316	Machine-learned electron correlation model based on frozen core approximation. *Journal of Chemical Physics*, **2020**, 153, 184108	3.9	4
315	Hierarchical parallelization of divide-and-conquer density functional tight-binding molecular dynamics and metadynamics simulations. *Journal of Computational Chemistry*, **2020**, 41, 1759-1772	3.5	3
314	Non-adiabatic molecular dynamics with divide-and-conquer type large-scale excited-state calculations. *Journal of Chemical Physics*, **2020**, 152, 224109	3.9	7
313	Quantum Chemical Reaction Prediction Method Based on Machine Learning. *Bulletin of the Chemical Society of Japan*, **2020**, 93, 685-693	5.1	7
312	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
311	Density-Functional Tight-Binding Study of Carbonaceous Species Diffusion on the (100)-□AlO Surface. *ACS Omega*, **2020**, 5, 6862-6871	3.9	4
310	Spin-flip approach within time-dependent density functional tight-binding method: Theory and applications. *Journal of Computational Chemistry*, **2020**, 41, 1538-1548	3.5	7
309	Heteroatom doping effects on interaction of HO and CeO (111) surfaces studied using density functional theory: Key roles of ionic radius and dispersion. *Journal of Chemical Physics*, **2020**, 152, 014707	3.9	9
308	Relativistic local hybrid functionals and their impact on 1s core orbital energies. *Journal of Chemical Physics*, **2020**, 152, 214103	3.9	4
307	Cover Image, Volume 10, Issue 1. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1459	7.9	
306	Confined water-mediated high proton conduction in hydrophobic channel of a synthetic nanotube. *Nature Communications*, **2020**, 11, 843	17.4	61
305	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
304	Large-scale excited-state calculation using dynamical polarizability evaluated by divide-and-conquer based coupled cluster linear response method. *Journal of Chemical Physics*, **2020**, 152, 024102	3.9	7
303	Weighted histogram analysis method for multiple short-time metadynamics simulations. *Chemical Physics Letters*, **2020**, 751, 137384	2.5	5
302	Catalytic Dehydrogenation of Ethane over Doped Perovskite via the Mars□an Krevelen Mechanism. *Journal of Physical Chemistry C*, **2020**, 124, 10462-10469	3.8	9

301	Solvent Selection Scheme Using Machine Learning Based on Physicochemical Description of Solvent Molecules: Application to Cyclic Organometallic Reaction. *Bulletin of the Chemical Society of Japan*, **2020**, 93, 841-845	5.1	5
300	Simulating the Coupled Structural-Electronic Dynamics of Photoexcited Lead Iodide Perovskites. *Journal of Physical Chemistry Letters*, **2020**, 11, 4448-4455	6.4	8
299	Finite-temperature-based time-dependent density-functional theory method for static electron correlation systems. *Journal of Chemical Physics*, **2020**, 152, 244111	3.9	0
298	Fast Nonadiabatic Molecular Dynamics via Spin-Flip Time-Dependent Density-Functional Tight-Binding Approach: Application to Nonradiative Relaxation of Tetraphenylethylene with Locked Aromatic Rings. *Journal of Chemical Theory and Computation*, **2020**, 16, 7299-7313	6.4	2
297	Hydroxide Ion Carrier for Proton Pumps in Bacteriorhodopsin: Primary Proton Transfer. *Journal of Physical Chemistry B*, **2020**, 124, 8524-8539	3.4	6
296	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
295	Recent advances in quantum-mechanical molecular dynamics simulations of proton transfer mechanism in various water-based environments. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1419	7.9	3
294	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	3.9	10
293	Unveiling controlling factors of the S/S minimum energy conical intersection (2): Application to penalty function method. *Journal of Chemical Physics*, **2020**, 152, 144108	3.9	5
292	Governing factors of supports of ammonia synthesis in an electric field found using density functional theory. *Journal of Chemical Physics*, **2019**, 151, 064708	3.9	9
291	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
290	Bond Energy Density Analysis Combined with Informatics Technique. *Journal of Physical Chemistry A*, **2019**, 123, 7777-7784	2.8	2
289	Efficient Semi-Numerical Implementation of Relativistic Exact Exchange within the Infinite-Order Two-Component Method Using a Modified Chain-of-Spheres Method. *Journal of Chemical Theory and Computation*, **2019**, 15, 4745-4763	6.4	11
288	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	6.4	10
287	Theoretical Analysis on Temperature- and Pressure-Dependences of NO-CO-O2 Reaction on Rh(111) Surface. *Journal of Computer Chemistry Japan*, **2019**, 18, 70-77	0.2	1
286	First-principle study of the oxidation mechanism of formaldehyde and hypophosphite for copper and nickel electroless deposition process. *Electrochimica Acta*, **2019**, 307, 536-542	6.7	9
285	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
284	Reversible Sodium Metal Electrodes: Is Fluorine an Essential Interphasial Component?. *Angewandte Chemie*, **2019**, 131, 8108-8112	3.6	2

283	Finite-temperature-based linear-scaling divide-and-conquer self-consistent field method for static electron correlation systems. *Chemical Physics Letters*, **2019**, 725, 18-23	2.5	8
282	Reversible Sodium Metal Electrodes: Is Fluorine an Essential Interphasial Component?. *Angewandte Chemie - International Edition*, **2019**, 58, 8024-8028	16.4	41
281	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
280	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
279	Extension and acceleration of relativistic density functional theory based on transformed density operator. *Journal of Chemical Physics*, **2019**, 150, 164104	3.9	6
278	Sodium- and Potassium-Hydrate Melts Containing Asymmetric Imide Anions for High-Voltage Aqueous Batteries. *Angewandte Chemie*, **2019**, 131, 14340-14345	3.6	8
277	Semi-local machine-learned kinetic energy density functional demonstrating smooth potential energy curves. *Chemical Physics Letters*, **2019**, 734, 136732	2.5	21
276	Virtual Reaction Condition Optimization based on Machine Learning for a Small Number of Experiments in High-dimensional Continuous and Discrete Variables. *Chemistry Letters*, **2019**, 48, 961-964	1.7	6
275	Restoring the iso-orbital limit of the kinetic energy density in relativistic density functional theory. *Journal of Chemical Physics*, **2019**, 151, 174114	3.9	5
274	Release of Relativistic Quantum Chemical Calculation Program RAQET. *Journal of Computer Chemistry Japan*, **2019**, 18, A6-A11	0.2	2
273	Theoretical Analysis of NO-CO Reaction Involving Lattice Oxygen. *Journal of Computer Chemistry Japan*, **2019**, 18, 139-141	0.2	
272	Development of Bond Energy Density Analysis with Informatics Technique. *Journal of Computer Chemistry Japan*, **2019**, 18, 152-155	0.2	
271	Quantum Mechanical Molecular Dynamics Simulations of Polaron Formation in a Perovskite Solar Cell Material. *Journal of Computer Chemistry Japan*, **2019**, 18, 142-144	0.2	1
270	Surface Reaction Simulation based on Divide-and-Conquer Type Density Functional Tight-Binding Molecular Dynamics (DC-DFTB-MD) Method´: Case for Proton Diffusion on Pt(111) Surface. *Vacuum and Surface Science*, **2019**, 62, 486-491	0	
269	Quantum mechanical molecular dynamics simulations of polaron formation in methylammonium lead iodide perovskite. *Physical Chemistry Chemical Physics*, **2019**, 22, 97-106	3.6	12
268	Relativistic Effect on Homogeneous Catalytic Reaction by Cationic Iridium Catalysts. *Journal of Computer Chemistry Japan*, **2019**, 18, 136-138	0.2	1
267	Spectroscopic and Computational Analyses of Liquid–Liquid Interfacial Reaction Mechanism of Boric Acid Esterification with 2,2,4-Trimethyl-1,3-pentanediol in Boron Extraction Processes. *Journal of Physical Chemistry C*, **2018**, 122, 10423-10429	3.8	3
266	Derivative of electron repulsion integral using accompanying coordinate expansion and transferred recurrence relation method for long contraction and high angular momentum. *International Journal of Quantum Chemistry*, **2018**, 118, e25640	2.1	4

265	Quantum chemical approach for condensed-phase thermochemistry (V): Development of rigid-body type harmonic solvation model. *Chemical Physics Letters*, **2018**, 700, 149-155	2.5	2
264	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
263	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
262	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
261	Simulations of the synthesis of boron-nitride nanostructures in a hot, high pressure gas volume. *Chemical Science*, **2018**, 9, 3803-3819	9.4	23
260	Gauge-origin independent formalism of two-component relativistic framework based on unitary transformation in nuclear magnetic shielding constant. *Journal of Chemical Physics*, **2018**, 148, 114109	3.9	6
259	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
258	Development of Divide-and-Conquer Density-Functional Tight-Binding Method for Theoretical Research on Li-ion Battery. *Chemical Record*, **2018**, 19, 746	6.6	5
257	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
256	Density-Functional Tight-Binding Molecular Dynamics Simulations of Excess Proton Diffusion in Ice I, Ice I, Ice III, and Melted Ice VI Phases. *Journal of Physical Chemistry A*, **2018**, 122, 33-40	2.8	12
255	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
254	Release of DCDFTBMD Program. *Journal of Computer Chemistry Japan*, **2018**, 17, A21-A27	0.2	2
253	Unveiling Controlling Factors of the S/S Minimum Energy Conical Intersection: A Theoretical Study. *Journal of Physical Chemistry A*, **2018**, 122, 8905-8910	2.8	9
252	Fractional-occupation-number based divide-and-conquer coupled-cluster theory. *Chemical Physics Letters*, **2018**, 712, 184-189	2.5	3
251	RAQET: Large-scale two-component relativistic quantum chemistry program package. *Journal of Computational Chemistry*, **2018**, 39, 2333-2344	3.5	13
250	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
249	Quantum chemical approach for positron annihilation spectra of atoms and molecules beyond plane-wave approximation. *Journal of Chemical Physics*, **2018**, 148, 184110	3.9	5
248	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

247	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
246	Development of spin-dependent relativistic open-shell Hartree□Fock theory with time-reversal symmetry (II): The restricted open-shell approach. *International Journal of Quantum Chemistry*, **2017**, 117, e25366	2.1	3
245	Development of spin-dependent relativistic open-shell Hartree□Fock theory with time-reversal symmetry (I): The unrestricted approach. *International Journal of Quantum Chemistry*, **2017**, 117, e25356	2.1	3
244	Systematic Investigation of the Thermodynamic Properties of Amine Solvents for CO2Chemical Absorption Using the Cluster-Continuum Model. *Bulletin of the Chemical Society of Japan*, **2017**, 90, 451-460	3.1	9
243	Relativistic effect on enthalpy of formation for transition-metal complexes. *Chemical Physics Letters*, **2017**, 673, 24-29	2.5	2
242	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
241	Decomposition of Effective Exchange Integrals of Radical Dimers Using Bond Energy Density Analysis. *Chemistry Letters*, **2017**, 46, 879-882	1.7	1
240	Relativistic density functional theory with picture-change corrected electron density based on infinite-order Douglas-Kroll-Hess method. *Chemical Physics Letters*, **2017**, 680, 37-43	2.5	10
239	Universal formulation of second-order generalized Mller□Plesset perturbation theory for a spin-dependent two-component relativistic many-electron Hamiltonian. *Chemical Physics Letters*, **2017**, 675, 137-144	2.5	5
238	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
237	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
236	Near-infrared absorption of □stacking columns composed of trioxotriangulene neutral radicals. *Npj Quantum Materials*, **2017**, 2,	5	41
235	Computerized implementation of higher-order electron-correlation methods and their linear-scaling divide-and-conquer extensions. *Journal of Computational Chemistry*, **2017**, 38, 2520-2527	3.5	8
234	A Linear-Scaling Divide-and-Conquer Quantum Chemical Method for Open-Shell Systems and Excited States **2017**, 297-321		2
233	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
232	Efficient pole-search algorithm for dynamic polarizability: Toward alternative excited-state calculation for large systems. *Journal of Computational Chemistry*, **2017**, 38, 7-14	3.5	4
231	Harmonic Solvation Model (HSM) for Evaluation of Condensed-Phase Free Energy. *Journal of Computer Chemistry Japan*, **2017**, 16, 83-88	0.2	
230	Informatics-Based Energy Fitting Scheme for Correlation Energy at Complete Basis Set Limit. *Journal of Computational Chemistry*, **2016**, 37, 2304-15	3.5	5

229	Relativistic frozen core potential scheme with relaxation of core electrons. *Chemical Physics Letters*, **2016**, 663, 97-103	2.5	3
228	Quantum chemical approach for condensed-phase thermochemistry (IV): Solubility of gaseous molecules. *Chemical Physics Letters*, **2016**, 655-656, 103-109	2.5	4
227	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	2.5	16
226	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
225	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
224	Electronic Transition Process of Fluorescence Appearing in Various Organic Polymers. *IEEJ Transactions on Fundamentals and Materials*, **2016**, 136, 205-211	0.2	
223	Development of Reaction Prediction Scheme Based on Machine Learning with Quantum Chemical Descriptors. *Journal of Computer Chemistry Japan*, **2016**, 15, 63-65	0.2	
222	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
221	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
220	Implementation of Analytical Energy Gradient of Spin-Dependent General Hartree-Fock Method Based on the Infinite-Order Douglas-Kroll-Hess Relativistic Hamiltonian with Local Unitary Transformation. *Journal of Chemical Theory and Computation*, **2016**, 12, 2181-90	6.4	7
219	The divide-and-conquer second-order proton propagator method based on nuclear orbital plus molecular orbital theory for the efficient computation of proton binding energies. *Physical Chemistry Chemical Physics*, **2016**, 18, 27422-27431	3.6	8
218	Initial Framework for Software Quality Evaluation Based on ISO/IEC 25022 and ISO/IEC 25023 **2016**,		4
217	Assessment of self-consistent field convergence in spin-dependent relativistic calculations. *Chemical Physics Letters*, **2016**, 657, 65-71	2.5	48
216	A divide-and-conquer method with approximate Fermi levels for parallel computations. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	5
215	Revisiting the extrapolation of correlation energies to complete basis set limit. *Journal of Computational Chemistry*, **2015**, 36, 1075-82	3.5	28
214	Accompanying coordinate expansion and recurrence relation method using a transfer relation scheme for electron repulsion integrals with high angular momenta and long contractions. *Journal of Chemical Physics*, **2015**, 142, 204110	3.9	5
213	Local response dispersion method: A density-dependent dispersion correction for density functional theory. *International Journal of Quantum Chemistry*, **2015**, 115, 309-324	2.1	10
212	Local response dispersion method in periodic systems: Implementation and assessment. *Journal of Computational Chemistry*, **2015**, 36, 303-11	3.5	2

211	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
210	Linearity condition for orbital energies in density functional theory (V): Extension to excited state calculations. *Chemical Physics Letters*, **2015**, 618, 30-36	2.5	3
209	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
208	Effect of Hartree-Fock exact exchange on intramolecular magnetic coupling constants of organic diradicals. *Journal of Chemical Physics*, **2015**, 142, 024318	3.9	17
207	Theoretical Analysis of the Oxidation Potentials of Organic Electrolyte Solvents. *ECS Electrochemistry Letters*, **2015**, 4, A103-A105		6
206	Quantum chemical approach for condensed-phase thermochemistry (II): Applications to formation and combustion reactions of liquid organic molecules. *Chemical Physics Letters*, **2015**, 624, 6-11	2.5	9
205	Large-scale two-component relativistic quantum-chemical theory: Combination of the infinite-order douglas□kroll□hess method with the local unitary transformation scheme and the divide-and-conquer method. *International Journal of Quantum Chemistry*, **2015**, 115, 253-257	2.1	5
204	Energy Expression of the Chemical Bond Between Atoms in Hydrides and Oxides and Its Application to Materials Design **2015**, 183-213		1
203	Acceleration of self-consistent field convergence in ab initio molecular dynamics simulation with multiconfigurational wave function. *Journal of Computational Chemistry*, **2014**, 35, 1473-80	3.5	2
202	Improving quasiparticle second order electron propagator calculations with the spin-component-scaled technique. *Chemical Physics Letters*, **2014**, 591, 82-87	2.5	9
201	Theoretical Study on the Selective Fluorescence of PicoGreen: Binding Models and Photophysical Properties. *Bulletin of the Chemical Society of Japan*, **2014**, 87, 267-273	5.1	2
200	DFT Analysis on Cathodic Reaction of Au Thiosulfate Complex at Au(111) Surface - Cathodic Reaction Modeling. *ECS Transactions*, **2014**, 58, 73-79	1	2
199	Extension of accompanying coordinate expansion and recurrence relation method for general-contraction basis sets. *Journal of Computational Chemistry*, **2014**, 35, 1517-27	3.5	4
198	Quantum chemical approach for condensed-phase thermochemistry: proposal of a harmonic solvation model. *Journal of Chemical Physics*, **2014**, 141, 174106	3.9	18
197	Frozen core potential scheme with a relativistic electronic Hamiltonian: Theoretical connection between the model potential and all-electron treatments. *Chemical Physics Letters*, **2014**, 592, 341-348	2.5	12
196	Large-Scale and Highly Accurate Relativistic Quantum-Chemical Scheme:toward Establishment ofTheoretical Foundation for Element Strategy. *Journal of Computer Chemistry Japan*, **2014**, 13, 1-17	0.2	5
195	4.??????????????????. *Electrochemistry*, **2014**, 82, 1098-1101	1.2	2
194	Accelerating convergence in the antisymmetric product of strongly orthogonal geminals method. *International Journal of Quantum Chemistry*, **2013**, 113, 239-244	2.1	19

193	Linearity condition for orbital energies in density functional theory (IV): Determination of range-determining parameter. *International Journal of Quantum Chemistry*, **2013**, 113, 245-251	2.1	6
192	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
191	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
190	Divide-and-conquer-based quantum chemical study for interaction between HIV-1 reverse transcriptase and MK-4965 inhibitor. *International Journal of Quantum Chemistry*, **2013**, 113, 510-517	2.1	8
189	Theoretical analysis of the influence of surface defects on the reactivity of hypophosphite ions. *Electrochimica Acta*, **2013**, 113, 785-791	6.7	11
188	Kinetic energy decomposition scheme based on information theory. *Journal of Computational Chemistry*, **2013**, 34, 2787-95	3.5	
187	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
186	Assessment of local response dispersion method for open-shell systems. *Chemical Physics Letters*, **2013**, 556, 386-392	2.5	9
185	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
184	Acceleration effect of thiourea on the oxidation reaction of hypophosphite ion on Ni surface. *Electrochimica Acta*, **2013**, 100, 311-316	6.7	11
183	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
182	Theoretical Study on Stability of Lithium Ion Battery in Charging Process: Analysis Based on Partial Charge and Partial Energy. *Journal of the Electrochemical Society*, **2013**, 160, A1364-A1368	3.9	3
181	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
180	Linearity condition for orbital energies in density functional theory (III): benchmark of total energies. *Journal of Computational Chemistry*, **2013**, 34, 1218-25	3.5	2
179	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
178	Divide-and-Conquer Electronic-Structure Study on the Mechanism of the West Nile Virus NS3 Protease Inhibitor. *Bulletin of the Chemical Society of Japan*, **2013**, 86, 67-74	5.1	4
177	Superphenalenyl: Theoretical Design of a □Conjugated Planar Hydrocarbon Radical. *Chemistry Letters*, **2013**, 42, 1386-1387	1.7	4
176	Evaluation of electron repulsion integral of the explicitly correlated Gaussian-nuclear orbital plus molecular orbital theory. *Chemical Physics Letters*, **2012**, 521, 142-149	2.5	12

175	Constrained self-consistent field method revisited toward theoretical designs of functional materials under external field. *Chemical Physics Letters*, **2012**, 530, 132-136	2.5	3
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