サブ課題A：新エネルギー源の創出・確保－太陽光エネルギー

サブ課題代表者：天能 精一郎

1. 学会誌・雑誌等における論文掲載

No.	掲載した論文（発表題目）	発表者氏名	発表した場所（学会誌・雑誌名等）	発表した時期	国内・国際の別	査読（有りの場合○を記入）
1	Explicitly correlated frequency-independent second-order Green's function for accurate ionization potentials	Yu-ya Ohnishi and Seiichiro Ten-no	J. Comput. Chem., 37 2447-2453 (2016)	2016年8月	国外	○
2	General technique for analytical derivatives of post-projected Hartree-Fock	Takashi Tsuchimochi and Seiichiro Ten-no	J. Chem. Phys., 146 074104 (2017)	2017年1月	国外	○
3	Perspective: Explicitly correlated electronic structure theory for complex systems	Andreas Grüneis, So Hirata, Yu-ya Onishi and Seiichiro Ten-no	J. Chem. Phys., 146 080901 (2017)	2017年2月	国外	○
4	Analytic energy gradient of projected Hartree-Fock within projection after variation	Motoyuki Uejima and Seiichiro Ten-no	J. Chem. Phys., 146 104106 (2017)	2017年3月	国外	○
5	Bridging Single- and Multireference Domains for Electron Correlation: Spin-Extended Coupled Electron Pair Approximation	Takashi Tsuchimochi and Seiichiro Ten-no	J. Chem. Theor. Comp., 13 1667-1681 (2017)	2017年2月	国外	○
6	"Theoretical study on the cooperative exciton dissociation process based on dimensional and hot charge-transfer state effects in an organic photocell"	T. Shimazaki, T. Nakajima	J. Chem. Phys. 144, 234906 (2016).	2016年6月	国外	○
7	"Large-scale QM/MM calculations of the CaMn4O5 cluster in the oxygen-evolving complex of photosystem II: Comparisons with EXAFS structures"	M. Shoji, H. Isobe, T. Nakajima, K. Yamaguchi	Chem. Phys. Lett. 658, 354-363 (2016).	2016年8月	国外	○
8	"Spectroscopic and computational study of acetic acid and its cyclic dimer in the near-infrared region"	K. B. Beć, Y. Futami, M. J. Wójcik, T. Nakajima, Y. Ozaki	J. Phys. Chem. A 120, 6170—6183 (2016).	2016年8月	国外	○
9	"Application of the dielectric-dependent screened exchange potential approach to organic photocell materials"	T. Shimazaki, T. Nakajima	Phys. Chem. Chem. Phys. 18, 27554—27563 (2016). DOI: 10.1039/C6CP04863C	2016年9月	国外	○
10	"Massively parallel algorithm and implementation of RI-MP2 energy calculation for peta-scale many-core supercomputers"	M. Katouda, A. Naruse, Y. Hirano, T. Nakajima	J. Comput. Chem. 37, 2623—2633 (2016). DOI: 10.1002/jcc.24491	2016年9月	国外	○
11	"Quantum chemical calculations of basic molecules: alcohols and carboxylic acids"	K. B. Beć, M. J. Wójcik, T. Nakajima	NIR news, 27(8), 15—21 (2016). DOI: 10.1255/nirn.1650	2016年11月	国外	○
12	"酢酸−リン酸アニオンクラスターの分子間水素結合における核の量子揺らぎの効果に関する理論的研究"	川島雪生, 澤田啓介, 中嶋隆人, 立川仁典	J. Comput. Chem. Japan, 15, 203—209 (2016). http://doi.org/10.2477/jccj.2016-0043	2016年12月	国内	○
13	MPI/OpenMP hybrid parallel algorithm for resolution of identity second-order Møller-Plesset perturbation calculation of analytical energy gradient for massively parallel multicore supercomputers	M. Katouda, T. Nakajima	J. Comput. Chem. 38, 489-507 (2017). DOI: 10.1002/jcc.24701	2017年1月	国外	○

14	Two-component relativistic equation-of-motion coupled-cluster methods for excitation energies and ionization potentials of atoms and molecules	Y. Akinaga, T. Nakajima	J. Phys. Chem. A 121, 827-835 (2017). DOI: 10.1021/acs.jpca.6b10921	2017年1月	国外	○
15	Group molecular orbital approach to solve the Huzinaga subsystem self-consistent-field equations	T. Shimazaki, K. Kitaura, D. Fedorov, T. Nakajima	J. Chem. Phys. 146, 084109 (2017). doi: http://dx.doi.org/10.1063/1.4976646	2017年2月	国外	○
16	Electrical anharmonicity in hydrogen bonded systems. Complete interpretation of the IR spectra of Cl-H stretching band in the gaseous (CH3)2O...HCl complex	N. Rekik, J. Suleiman, M. J. Wójcik, H. T. Flakus, T. Nakajima	Phys. Chem. Chem. Phys. 19, 5917-5931 (2017).	2017年1月	国外	○
17	Large-scale QM/MM calculations of the CaMn4O5 cluster in the S3 state of the oxygen evolving complex of photosystem II. Comparison between water-inserted and no water-inserted structures	M. Shoji, H. Isobe, T. Nakajima, Y. Shigeta, M. Suga, F. Akita, J.-R. Shen, K. Yamaguchi	Faraday Discussions 198, 83-106 (2017).	2016年11月	国外	○
18	Infrared spectroscopy and Born-Oppenheimer molecular dynamics simulation study on deuterium substitution in the crystalline benzoic acid	M. Gług, M. Brela, M. Boczar, A. Turek, Ł. Boda, M. Wójcik, T. Nakajima, Y. Ozaki	J. Phys. Chem. B 121, 479-489 (2017).	2016年12月	国外	○
19	″Dipole Analyses for Short-Circuit Current in Organic Photovoltaic Devices of Diketopyrrolopyrrole-Based Donor and PCBM″	Shohei Koda, Mikiya Fujii, Shintaro Hatamiya, Koichi Yamashita	Theor. Chem. Acc., 135(5), 115 - 124	2016年4月	国外	○
20	″The Effects of the Organic-Inorganic Interactions on the Thermal Transport Properties of CH3NH3PbI3″	Tomoyuki Hata, Giacomo Giorgi, Koichi Yamashita	Nano Lett., 2016, 16 (4), pp 2749-2753	2016年4月	国外	○
21	″Atomic-scale analysis of the RuO_2/water interface under electrochemical conditions″	E. Watanabe, J. Rossmeisl, M. Bjorketun, H. Ushiyama, K. Yamashita	J. Phys. Chem. C, 120, 8096-8103	2016年4月	国外	○
22	″A new implementation of ab initio Ehrenfest dynamics using electronic configuration basis - exact formulation with molecular orbital connection and effective propagation scheme	Tomotaka Kunisada, Hiroshi Ushiyama, Koichi Yamashita	Int. J. Quant. Chem., 116, 1205-1213	2016年5月	国外	○
23	“Proton Transfer Dynamics in Protonated Benzene”	Ayaka Kuroki, Hiroshi Ushiyama, Koichi Yamashita	Bull. Chem. Soc. Japan, 89, 804-809	2016年7月	国外	○
24	“Theoretical studies on ammonia borane dehydrogenation catalyzed by iron pincer complexes”	Ayaka Kuroki, Hiroshi Ushiyama, Koichi Yamashita	Computational and Theoretical Chemistry, 1090, 214-217	2016年8月	国外	○
25	“Does Organic/Organic Interface Mimic Band Bending by Deforming Structure?”	Ryota Jono, Eriko Watanabea, Mikiya Fujii, Koichi Yamashita	J. of Photochem. Photobio. A: Chemistry, 330, 181-185	2016年8月	国外	○
26	“Structural and electronic features of small hybrid organic-inorganic halide perovskite clusters: a theoretical analysis”	Giacomo Giorgi, Tomohiro Yoshihara, Koichi Yamashita	Phys. Chem. Chem. Phys., DOI: 10.1039/c6cp03193e	2016年9月	国外	○
27	“Thermal Effect on Morphology and Performance of Organic Photovoltaics”	E. Kawashima, M. Fujii, K. Yamashita	Phys. Chem. Chem. Phys., 18, 26456 - 26465	2016年9月	国外	○
28	″Photon-absorbing charge-bridging states in organic bulk heterojunctions consisting of diketopyrrolopyrrole derivatives and PCBM″	Mikiya Fujii, Woong Shin, Takuma Yasuda, Koichi Yamashita	Phys Chem Chem Phys, 18(14), 9514 -9523	2016年10月	国外	○

29	″Anion Ordering in $CaTaO_2N$: Structural Impact on the Photocatalytic Activity. Insights from First-Principles″	Ayako Kubo, Giacomo Giorgi, Koichi Yamashita	Chem Mater., 29, 539-545	2016年12月	国外	○
30	″Charge Carrier Trapping at Surface Defects of Perovskite Solar Cell Absorbers: A First-Principles Study″	Hiroki Uratani, Koichi Yamashita	J. Phys. Chem. Lett., 8, 742-746	2017年1月	国外	○
31	″On the development of a classical interatomic potential for MAPbBr″	Tomoyuki Hata, GiacomoGiorgi,Claudia Caddeo,Alessandro Mattoni, KoichiYamashita	J. Phys. Chem. C, 121, 3724-3733	2017年1月	国外	○
32	“Defects in crystalline PVDF: a Density Functional Theory – Density Functional Tight Binding study”	Saeid Arabnejad, Koichi Yamashita, Sergei Manzhos	Phys. Chem. Chem. Phys., 19, 7560-7567	2017年2月	国外	○
33	“Synthesis of Quinoidal Fused Oligosiloles by Rhodium-Catalyzed Stitching Reaction and Theoretical Investigation of Their Properties”	Ryo Shintani, Nana Misawa, Tomohiro Tsuda, Ryo Iino, Mikiya Fujii, Koichi Yamashita, Kyoko Nozaki	J. Am. Chem. Soc., 139, 3861-3867	2017年2月	国外	○
34	″First-principles study of the band diagrams and Schottky-type barrier heights of aqueous Ta3N5 interfaces″	Eriko Watanabe, Hiroshi Ushiyama, Koichi Yamashita	ACS Appl. Mater. Interfaces, 9, 9559-9566	2017年3月	国外	○

サブ課題B:エネルギーの変換・貯蔵－電気エネルギー

サブ課題代表者:杉野 修

1. 学会誌・雑誌等における論文掲載

No.	掲載した論文（発表題目）	発表者氏名	発表した場所（学会誌・雑誌名等）	発表した時期	国内・国際の別	査読（有りの場合○を記入）
1	Ab-initio moleculer dynamics of solvation effects on reactiveity at electrified interfaces	J.A. Herron, Y. Morikawa, and M. Mavrikakis	Proc. Natl. Acad. Sci. U. S. A., 113, E4937-E4945 (2016)	2016年8月	国外	○
2	Superconcentrated electrolytes for a high-voltage lithium-ion battery	Jianhui Wang, Yuki Yamada, Keitaro Sodeyama, Ching Hua Chian, Yoshitaka Tateyama, Atsuo Yamada	Nat. Commun., 7, 12032 (2016)	2016年6月	国外	○
3	Catalytic Proton Dynamics at the Water/Solid Interface of Ceria Supported Pt Clusters	Matteo Farnesi Camellone, Fabio Negreiros Ribeiro, Lucie Szabova, Yoshitaka Tateyama, Stefano Fabris	J. Am Chem. Soc., 138, 11560-11567 (2016)	2016年7月	国外	○
4	Hydrate-melt electrolytes for high-energy-density aqueous batteries	Yuki Yamada, Kenji Usui, Keitaro Sodeyama, Seongjae Ko, Yoshitaka Yateyama, Atsuo Yamada	Nat. Energy, 13, 16129 (2016)	2016年8月	国外	○

5	The Solvation Structure of Lithium Ions in an Ether Based Electrolyte Solution from First-Principles Molecular Dynamics	Martin Callsen, Keitaro Sodeyama, Zdenek Futera, Yoshitaka Tateyama, Ikutaro Hamada	J. Phys. Chem. B, 121 (2016)	2016年12月	国外	○
6	Cation Mixing Properties toward Co Diffusion at the $LiCoO_2$ Cathode/ Sulfide Electrolyte Interface in a Solid-State Battery	Jun Haruyama, Keitaro Sodeyama, Yoshitaka Tateyama	ACS Appl. Mater. Interfaces (2016)	2016年12月	国外	○
7	Enhanced Li-Ion Accessibility in MXene Titanium Carbide by Steric Chloride Termination	Satoshi Kajiyama, Lucie Szabova, Hiroki Iinuma, Akira Sugahara, Kazuma Gotoh, Keitaro Sodeyama, Yoshitaka Tateyama, Masashi Okubo, Atsuo Yamada	Adv. Energy Mater., 1601873(2017)	2017年1月	国外	○
8	An Active Site Opening Mechanism in Ion Pair of (pyridylamide) Hf(IV) Catalyst: An Associative Mechanism	K. Matsumoto, K. S. Sandhya, M. Takayanagi, N. Koga, M. Nagaoka	Organometallics, 35 (24) 4099-4105 (2016) DOI: 10.1021/acs.organomet.6b00804	2016年12月	国外	○
9	Na+ Binding Is Ineffective in Forming a Primary Substrate Pocket of Thrombin	I. Kurisaki, M. Nagaoka	The Journal of Physical Chemistry B, 120 (46) 11873-11879 (2016) DOI: 10.1021/acs.jpcb.6b07827	2016年5月	国外	○
10	Formation of Reactant Complex Structure for Initiation Reaction of Lactone Ring-Opening Polymerization by Cooperation of Multiple Cyclodextrin	M.Takayanagi, S.Ito, K.Matsumoto, M.Nagaoka	The Journal of Physical Chemistry B, 120 (29) 7174-7181 (2016) DOI: 10.1021/acs.jpcb.6b04372	2016年7月	国外	○
11	Additive Effect of Fluoroethylene and Difluoroethylene Carbonates for the Solid Electrolyte Interphase Film Formation in Sodium-Ion Batteries: A Quantum Chemical Study	U.Purushotham, N.Takenaka, M.Nagaoka	RSC Advances,6、65232-65242(2016) DOI: 10.1039/C6RA09560G	2016年7月	国外	○
12	Revisiting the Stereochemistry of Propylene Isotactic Polymerization Reaction Mechanism on C2 symmetric $[SiH_2(Ind)_2ZrCH_3]+$ and $[SiH_2(Ind)_2ZrCH_3]+[CH_3B(C_6F_5)_3]-$	S.K. Sankaran, N.Koga, M.Nagaoka	Bulletin of the Chemical Society of Japan, 89 1093-1105 (2016) DOI:http://dx.doi.org/10.1246/bcsj.20160119	2016年6月	国外	○
13	The Bound Na+ is Negative Effecter for Thrombin-Substrate Stereospecific Complex Formation	I.Kurisaki, M.Takayanagi, M.Nagaoka	The Journal of Physical Chemistry B, 120 (20) 4540-4547 (2016) DOI: 10.1021/acs.jpcb.6b00976	2016年5月	国外	○
14	Evaluation of atomic pressure in the multiple time-step integration algorithm	Y Andoh, A. Yamada, N. Yoshii, S Okazaki	J. Comput. Chem.	2017年1月	国外	○
15	Detailed structural analysis of a self-assembled vesicular amphiphilic NCN-pincer Palladium complex by using wide-angle X-ray scattering and molecular dynamics calculations	G. Hamasaka, T. Muto, Y. Andoh, K. Fujimoto, K. Kato, M. Takata, S. Okazaki, Y. Uozumi	Chemistry-A European Journal	2016年12月	国外	○

16	A molecular dynamics study of local pressures and interfacial tensions of SDS micelles and dodecane droplets in water micelles and dodecane droplets in water	Masahiro Kitabata, Kazushi Fujimoto, Noriyuki Yoshii, and Susumu Okazaki	J. Chem. Phys.	2016年6月	国外	○
17	Molecular Dynamics Study of the Morphology of Hydrated Perfluorosulfonic Acid Polymer Membranes	An-Tsung Kuo, Wataru Shinoda, and Susumu Okazaki	J. Phys. Chem. C, 2016, 120 (45), pp 25832-25842 DOI: 10.1021/acs.jpcc.6b08015	2016年10月	国外	○

サブ課題C:エネルギー・資源の有効利用－化学エネルギー

サブ課題代表者:田中 秀樹

1. 学会誌・雑誌等における論文掲載

No.	掲載した論文(発表題目)	発表者氏名	発表した場所(学会誌・雑誌名等)	発表した時期	国内・国際の別	査読(有りの場合○を記入)
1	Formation of clathrate hydrates of water-soluble guest molecules	Takuma Yagasaki, Masakazu Matsumoto, Hideki Tanaka	J. Phys. Chem. C. 120. 21512-21521 (2016)	2016年9月	国外	○
2	Exploring the Mechanism of Ultrafast Intersystem Crossing in Re(I) Carbonyl Bipyridine Halide Complexes: Key Vibrational Modes and Spin-Vibronic Quantum Dynamics	Y. Harabuchi, J. Eng, E. Gindensperger, T. Taketsugu, S. Maeda, and C. Daniel	J. Chem. Theo. Comp., 12, 2335-2345 (2016).	2016年4月	国外	○
3	Core-Structure-Dependent Luminescence of Thiolato-Bridged Copper(I) Cluster Complexes	K. Shimada, A. Kobayashi, Y. Ono, H. Ohara, T. Hasegawa, T. Taketsugu, E. Sakuda, S. Akagi, N. Kitamura, and M. Kato	J. Phys. Chem. C, 120, 16002-16011 (2016).	2016年4月	国外	○
4	Highly Active and Robust Metalloporphyrin Catalysts for the Synthesis of Cyclic Carbonates from a Broad Range of Epoxides and Carbon Dioxide	Maeda Chihiro, Shimonishi Junta, Miyazaki Ray, Hasegawa Jun-ya, Ema Tadashi	Chemistry, Eur. J. 22, 6556-6563 (2016).	2016年5月	国外	○
5	Nonadiabatic Pathways of Furan and Dibenzofuran: What Makes Dibenzofuran Fluorescent?	Y. Harabuchi, T. Taketsugu, and S. Maeda	Chem. Lett., 45, 940-942 (2016).	2016年5月	国外	○
6	Theoretical Study of Hydrogenation Catalysis of Phosphorus Compound and Prediction of Catalyst with High Activity and Wide Application Scope	G. Zeng, S. Maeda, T. Taketsugu, and S. Sakaki	ACS Catal., 6, 4859-4870 (2016).	2016年5月	国外	○
7	Structural dynamics of photochemical reactions probed by time-resolved photoelectron spectroscopy using high harmonic pulse	R. Iikubo, T. Sekikawa, Y. Harabuchi, and T. Taketsugu	Faraday Discuss., 194, 147-160 (2016).	2016年5月	国外	○
8	Theoretical study on mechanism of the photochemical ligand substitution of fac-[ReI(bpy)(CO)3(PR3)]+ complex	K. Saita, Y. Harabuchi, T. Taketsugu, O. Ishitani, and S. Maeda	Phys. Chem. Chem. Phys., 18, 17557-17564 (2016).	2016年6月	国外	○
9	Artificial Force Induced Reaction (AFIR) Method for Exploring Quantum Chemical Potential Energy Surfaces	S. Maeda, Y. Harabuchi, M. Takagi, T. Taketsugu, and K. Morokuma	Chem. Rec., 16, 2232-2248 (2016).	2016年6月	国外	○

10	A DFT and Multi-configurational Perturbation Theory Study on O_2 Binding to a Model Heme Compound via the Spin-change Barrier	Y. Kitagawa, Y. Chen, N. Nakatani, A. Nakayama, and J. Hasegawa	Phys. Chem. Chem. Phys. 18, 18137-18144 (2016).	2016年7月	国外	○
11	When inert becomes active: fascinating route for catalyst design	A. Lyalin, M. Gao, and T. Taketsugu	Chem. Rec., 16, 2324-2337 (2016).	2016年7月	国外	○
12	Spin-blocking effect in CO and H_2 binding reactions to molybdenocene and tungstenocene: A theoretical study on the reaction mechanism via minimum energy intersystem-crossing	K. Watanabe, N. Nakatani, A. Nakayama, M. Higashi, and J. Hasegawa	Inorg. Chem. 55, 8082-8090 (2016).	2016年8月	国外	○
13	Divide-and-Conquer Hartree-Fock-Bogoliubov Method and Its Application to Conjugated Diradical Systems	M. Kobayashi and T. Taketsugu	Chem. Lett., 45, 1268-1270 (2016).	2016年8月	国外	○
14	Highly Efficient Electrochemical Hydrogen Evolution Reaction at Insulating Boron Nitride Nanosheet on Inert Gold Substrate	K. Uosaki, G. Elumalai, H. C. Dinh, A. Lyalin, T. Taketsugu, and H. Noguchi	Scientific Reports, 6, 32217 (2016).	2016年8月	国外	○
15	Multi-Step Intersystem Crossing Pathways in Cinnamate-Based UV-B Sunscreens	K. Yamazaki, Y. Miyazaki, Y. Harabuchi, T. Taketsugu, S. Maeda, Y. Inokuchi, S.-n. Kinoshita, M. Sumida, Y. Onitsuka, H. Kohguchi, M. Ehara, and T. Ebata	J. Phys. Chem. Lett., 7, 4001-4007 (2016).	2016年9月	国外	○
16	Catalytic Hydrogenation of Carbon Dioxide with Ammonia-Borane by Pincer-type Phosphorus Compound: A Theoretical Prediction	G. Zeng, S. Maeda, T. Taketsugu, and S. Sakaki	J. Am. Chem. Soc. (Communication), 138, 13481-13484 (2016).	2016年10月	国外	○
17	Theoretical Study on Highly Active Bifunctional Metalloporphyrin Catalysts for the Coupling Reaction of Epoxides with Carbon Dioxide	J. Hasegawa, R. Miyazaki, C. Maeda, and T. Ema	Chem. Rec. 16 2260-2267 (2016).	2016年10月	国外	○
18	Ab initio Molecular Dynamics Study of H_2 Formation Inside POSS Compounds. 2. The Effect of an Encapsulated Hydrogen Molecule	T. Kudo, T. Taketsugu, and M. S. Gordon	J. Phys. Chem. A, 120, 8699-8715 (2016).	2016年10月	国外	○
19	Ab Initio Molecular Dynamics Study of the Photoreaction of 1,1′ -Dimethylstilbene Upon S0 → S1 Excitation	Y. Harabuchi, R. Yamamoto, S. Maeda, S. Takeuchi, T. Tahara, and T. Taketsugu	J. Phys. Chem. A, 120, 8804-8812 (2016).	2016年10月	国外	○
20	Full Rate Constant Matrix Contraction Method for Obtaining Branching Ratio of Unimolecular Decomposition	Y. Sumiya, T. Taketsugu, and S. Maeda	J. Comp. Chem., 38, 101-109 (2017).	2016年10月	国外	○
21	Atomically thin hexagonal boron nitride nanofilm for Cu protection: The importance of film perfection	M. H. Khan, S. S. Jamali, A. Lyalin, P. J. Molino, L. Jiang, H. K. Liu, T. Taketsugu, and Z. Huang	Adv. Mater., 29, 1603937 (2017).	2016年11月	国外	○
22	Electronic Polarization Effect of the Water Environment in Charge-Separated Donor-Acceptor Systems: An Effective Fragment Potential Model Study	Kazuma Yanai, Kazuya Ishimura, Akira Nakayama, Michael Schmidt, Mark Gordon, Jun-ya Hasegawa	J. Phys. Chem. A 120, 10273-10280 (2016)	2016年12月	国外	○

23	Isomerization in Gold Clusters upon O_2 Adsorption	M. Gao, D. Horita, Y. Ono, A. Lyalin, S. Maeda, and T. Taketsugu	J. Phys. Chem. C, 121, 2661-2668 (2017).	2017年1月	国外	○
24	Interface Effects in Hydrogen Elimination Reaction from Isopropanol by Ni13 Cluster on θ-Al2O3(010) Surface	A. Lyalin, K. Shimizu, and T. Taketsugu	J. Phys. Chem. C, 121, 3488-3495 (2017).	2017年1月	国外	○
25	Two-Dimensional Corrugated Porous Carbon-, Nitrogen-Framework/Metal Heterojunction for Efficient Multi-Electron Transfer Processes with Controlled Kinetics	K. Sakaushi, A. Lyalin, S. Tominaka, T. Taketsugu, and K. Uosaki	ACS Nano, 11, 1770-1779 (2017).	2017年1月	国外	○
26	Combined Gradient Projection / Single Component Artificial Force Induced Reaction (GP/SC-AFIR) Method for an Efficient Search of Minimum Energy Conical Intersection (MECI) Geometries	Y. Harabuchi, T. Taketsugu, and S. Maeda	Chem. Phys. Lett., 674, 141-145 (2017).	2017年2月	国外	○
27	Density matrix renormalization group (DMRG) method as a common tool for large active-space CASSCF/CASPT2 calculations	N. Nakatani and S. Guo	J. Chem. Phys., 146, 094102 (2017)	2017年2月	国外	○
28	Thermally activated delayed fluorescence OLEDs with fully solution processed organic layers exhibiting nearly 10% external quantum efficiency	K. Albrecht, K. Matsuoka, D. Yokoyama, Y. Sakai, A. Nakayama, K. Fujita, and K. Yamamoto	Chem. Commun., 53, 2439-2442 (2017)	2017年2月	国外	○
29	Implementation of Analytical Energy Gradient of Spin-Dependent General Hartree-Fock Method Based on the Infinite-Order Douglas-Kroll-Hess Relativistic Hamiltonian with	Yuya Nakajima, Junji Seino, Hiromi Nakai	J. Chem. Theory Comput. 12, 2181 (2016)	2016年4月	国外	○
30	Quantum chemical approach for condensed-phase thermochemistry (IV): Solubility of gaseous molecules	Atsushi Ishikawa, Masahiro Kamata, Hiromi Nakai	Chem. Phys. Lett. 655-656, 103 (2016)	2016年5月	国外	○
31	Assessment of self-consistent field convergence in spin-dependent relativistic calculations	Masahiko Nakano, Junji Seino, Hiromi Nakai	Chem. Phys. Lett. 657, 65 (2016)	2016年5月	国外	○
32	Three pillars for achieving quantum mechanical molecular dynamics simulations of huge systems: Divide-and-conquer, density-functional tight-binding, and massively parallel computation	Hiroaki Nishizawa, Yoshifumi Nishimura, Masato Kobayashi, Stephan Irle, Hiromi Nakai	J. Comput. Chem. 37, 1983 (2016)	2016年6月	国外	○
33	Quantum chemistry beyond Born-Oppenheimer approximation on a quantum computer: A simulated phase estimation study	Libor Veis, Jakub Visnak, Hiroaki Nishizawa, Hiromi Nakai, Jiri Pittner	Int. J. Quantum Chem. 116, 1328 (2016)	2016年6月	国外	○
34	CO_2化学吸収法に対する計算化学研究:エネルギー・環境問題への挑戦	寺西慶, 石川敦之, 中井浩巳	J. Comput. Chem. Jpn. 15, A15 (2016)	2016年7月	国内	○
35	Informatics-Based Energy Fitting Scheme for Correlation Energy at Complete Basis Set Limit	Junji Seino, Hiromi Nakai	J. Comput. Chem. 37, 2304 (2016)	2016年7月	国外	○
36	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	Yusuke Tsukamoto, Yasuhiro Ikabata, Jonathan Romero, Andres Reyes, Hiromi Nakai	Phys. Chem. Chem. Phys. 18, 27422 (2016)	2016年9月	国外	○

37	Relativistic frozen core potential scheme with relaxation of core electrons	Yuya Nakajima, Junji Seino, Masao Hayami, Hiromi Nakai	Chem. Phys. Lett. 663, 97 (2016)	2016年9月	国外	○
38	Efficient pole-search algorithm for dynamic polarizability: Toward alternative excited-state calculation for large systems	Hiromi Nakai, Takeshi Yoshikawa, Yutaro Nonaka	J. Comput. Chem. 38, 7 (2017)	2016年10月	国外	○
39	量子化学計算情報を記述子とした機械学習に基づく反応予測手法の開発	藤波美起登, 清野淳司, 中井浩巳	J. Comput. Chem. Jpn. 15, 63 (2016)	2016年10月	国内	○
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