サブ課題C:エネルギー・資源の有効利用ー化学エネルギー

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 point	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.	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 Local Unitary Transformation	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	○

40	Implementation of Efficient Two-component Relativistic Method Using Local Unitary Transformation to GAMESS Program	Yuya Nakajima, Junji Seino, Michael W. Schmidt, Hiromi Nakai	J. Comput. Chem. Jpn. 15, 68 (2016)	2016年10月	国内	○
41	核・電子軌道法における原子核軌道エネルギーとプロトン束縛エネルギー計算	五十幡康弘, 中井浩巳	J. Comput. Chem. Jpn. 15, 148 (2016)	2016年10月	国内	○
42	Theoretical Analysis of Interactions between Potassium Ions and Organic Electrolyte Solvents: A Comparison with Lithium, Sodium, and Magnesium Ions	Masaki Okoshi, Yuki Yamada, Shinichi Komaba, Atsuo Yamada, Hiromi Nakai	J. Electrochem. Soc. 164, A54 (2017)	2016年12月	国外	○
43	Development of spin-dependent relativistic open-shell Hartree-Fock theory with time-reversal symmetry (I): The unrestricted approach	M. Nakano, J. Seino, H. Nakai	Int. J. Quantum Chem., 117 (10), e25356 (9 pages) (2017)	2017年1月	国外	○
44	Divide-and-conquer-type density-functional tight-binding simulations of hydroxide ion diffusion in bulk water	A. W. Sakti, Y. Nishimura, H. Nakai	J. Phys. Chem. B, 121 (6), 1362-1371 (2017)	2017年1月	国外	○
45	Systematic investigation of thermodynamic properties of amine solvents for CO_2 chemical absorption Using the cluster-continuum model	K. Teranishi, A. Ishikawa, H. Sato, H. Nakai	Bull. Chem. Soc. Jpn., 90 (4), 451-460 (2017)	2017年1月	国外	○
46	Unveiling a new aspect of simple aryboronic esters: Long-lived room-temperature phosphorescence from the heavy atom-free molecules	Y. Shoji, Y. Ikabata, Q. Wang, D. Nemoto, A. Sakamoto, N. Tanaka, J. Seino, H. Nakai, T. Fukushima	J. Am. Chem. Soc., 139 (7), 2728-2733 (2017)	2017年1月	国外	○
47	Relativistic effect on enthalpy of formation for transition-metal complexes	Y. Nakajima, J. Seino, H. Nakai	Chem. Phys. Lett., 673, 24-29 (2017)	2017年1月	国外	○
48	Development of spin-dependent relativistic open-shell Hartree-Fock theory with time-reversal symmetry (II): The restricted open-shell approach	M. Nakano, Nakamura, J. Seino, H. Nakai	Int. J. Quantum Chem., 117 (10), e25366 (12 pages) (2017)	2017年2月	国外	○
49	Universal formulation of second-order generalized Møller-Plesset perturbation theory for a spin-dependent two-component relativistic many-electron Hamiltonian	M. Nakano, J. Seino, H. Nakai	Chem. Phys. Lett., 675, 137-144 (2017)	2017年3月	国外	○
50	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	H. Nakai, T. Yoshikawa	J. Chem. Phys., 146 (12), 124123 (12 pages) (2017)	2017年3月	国外	○
51	Decomposition of effective exchange integrals of radical dimers using bond energy density analysis	Y. Ikabata, H. Nakai	Chem. Lett.10.1246/cl.170208(2017)	2017年3月	国外	○
52	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 W. Schmidt, Mark S. Gordon, and Jun-ya Hasegawa	J. Phys. Chem. A, 120, 10273-10280 (2016).	2016年11月	国外	○
53	Intel Xeon Phi上でのSMASHによる並列化DFT計算の性能評価	齊藤 天菜, 望月 祐志, 山崎 大, 石村 和也	J. Comput. Chem. Jpn., 15, 92-96 (2016).	2016年11月	国内	○