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	Configuration interaction combined with spin-projection for strongly correlated molecular electronic structures	Takashi Tsuchimochi, Seiichiro Ten-no	J. Chem. Phys. (communications), 144, 011101 (2016)	2016年1月	国外	○
2	Black-Box Description of Electron Correlation with the Spin-Extended Configuration Interaction Model: Implementation and Assessment	Takashi Tsuchimochi, Seiichiro Ten-no	J. Chem. Theor. Comp., 12, 1741-1759 (2016)	2016年3月	国外	○
3	Spin-flip configuration interaction singles with exact spin-projection: Theory and applications to strongly correlated systems	Takashi Tsuchimochi	J. Chem. Phys. 143, 144114 (2015)	2015年8月	国外	○
4	From C60 to Infinity: Large-Scale Quantum Chemistry Calculations of the Heats of Formation of Higher Fullerenes	B. Chan, Y. Kawashima, M. Katouda, T. Nakajima, K. Hirao	J. Am. Chem. Soc. 138, 1420-1429 (2016).	2016年1月	国外	○
5	Theoretical Study on Spin-Forbidden Transitions of Osmium Complexes by Two-component Relativistic Time-dependent Density Functional Theory	Y. Imamura, M. Kamiya, T. Nakajima	Chem. Phys. Lett. 648, 60-65 (2016).	2016年1月	国外	○
6	Gaussian-based range-separation approach on Hartree-Fock exchange interaction and second-order perturbation theory	T. Shimazaki, T. Nakajima	Chem. Phys. Lett. 647, 132-138 (2016).	2016年3月	国外	○
7	Full Geometry Optimizations of the CaMn4O4 Model Cluster for the Oxygen Evolving Complex of Photosystem II	M. Shoji, H. Isobe, T. Nakajima, K. Yamaguchi	Chem. Phys. Lett. 640, 23-30 (2015).	2015年11月	国外	○
8	Two-component Relativistic Time-dependent Density Functional Theory Study on Spin-forbidden Transitions for Metal Polypyridyl Complexes	Y. Imamura, M. Kamiya, T. Nakajima	Chem. Phys. Lett. 635, 152-156 (2015).	2015年8月	国外	○
9	Gaussian-based cutoff scheme on Hartree-Fock exchange term of dielectric-dependent potential	T. Shimazaki, T. Nakajima	Chem. Phys. Lett. 634, 83-87 (2015).	2015年8月	国外	○
10	How Can We Understand Au8 Cores and Entangled Ligands of Selenolate- and Thiolate-protected Gold Nanoclusters Au24(ER)20 and Au20(ER)16 (E = Se, S; R = Ph, Me)? A Theoretical Study	N. Takagi, K. Ishimura, M. Matsui, R. Fukuda, T. Matsui, T. Nakajima, M. Ehara, S. Sakaki	J. Am. Chem. Soc. 137, 8593-8602 (2015).	2015年6月	国外	○
11	Theoretical study of exciton dissociation through hot states at donor-acceptor interface in organic photocell	T. Shimazaki, T. Nakajima	Phys. Chem. Chem. Phys. 17, 12538 (2015).	2015年4月	国外	○
12	マルチGPU超並列クラスタシステムを用いた大規模ナノ炭素分子の電子状態計算	河東田道夫, 成瀬彰, 中嶋隆人	TSUBAME ESJ, 14, 14-18 (2016).	2016年3月	国内	
13	Dipole Analyses for Short-Circuit Current in Organic Photovoltaic Devices of Diketopyrrolopyrrole-Based Donor and PCBM	Shohei Koda, Mikiya Fujii, Shintaro Hatamiya, Koichi Yamashita	Theoret. Chem. Acc., 135, 115 (10 pages) (2016)	2016年3月	国外	○

14	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, 9514-9523 (2016)	2016年3月	国外	○
15	Zero-Dimensional Hybrid Organic—Inorganic Halide Perovskite Modeling: Insights from First Principles Giacomo Giorgi, Koichi Yamashita	Giacomo Giorgi, Koichi Yamashita	J. Phys. Chem. Lett., 7, 888-899 (2016)	2016年2月	国外	○
16	Remarkable Dependence of the Final Charge Separation Efficiency on the Donor-Acceptor Interaction in Photoinduced Electron Transfer	Tomohiro Higashino, Tomoki Yamada, Masanori Yamamoto, Akihiro Furube, Nikolai V. Tkachenko, Taku Miura, Yasuhiro Kobori, Ryota Jono, Koichi Yamashita, Hiroshi Imahori	Angewandte Chemie, 55, 629-633 (2016)	2015年12月	国外	○
17	Energy Alignment of Frontier Orbitals and Suppression of Charge Recombinations in P3HT/SWNT	Katsuhiko Nishimra, Mikiya Fujii, Ryota Jono, Koichi Yamashita	J. Phys. Chem. C, 119, 26258-26265 (2015)	2015年11月	国外	○
18	Zero-dipole molecular organic cations in mixed organic-inorganic halide perovskites: possible chemical solution for the reported anomalous hysteresis in the current-voltage curve measurements	G. Giorgi, K. Yamashita	Nanotechnology, 26, 442001 (16 pages) (2015)	2015年10月	国外	○
19	″Analyses on thiophene-based donor-acceptor semiconducting polymers toward designing optical and conductive properties: A theoretical perspective″	T. Matsui, Y. Imamura, I. Osaka, K. Takimiya, T. Nakajima	J. Phys. Chem. C, 120, 8305-8314 (2016).	2016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	Assessing the accuracy of the van der Waal density functionals for rare gas and molecular systems	M. Callsen and I. Hamada	Phys. Rev. B 91, 195103	2015年5月	国外	○
2	A single-atom-thick TiO_2 nanomesh on an insulating oxide	T. Ohsawa, M. Saito, I. Hamada, R. Shimizu, K. Iwaya, S. Shiraki, Z. Wang, Y. Ikuhara, T. Hitosugi	ACS Nano 9, 8766-8772	2015年8月	国外	○
3	Recent progress in predicting structural and electronic properties of organic solids with the van der Waals density functional	S. Yanagisawa, K. Okumura, T. Inaoka, and I. Hamada	J. Electron Spectrosc. Relat. Phenom. 204, 159-167	2015年10月	国外	○

4	Tuning the van der Waals Interaction of Graphene with Molecules via Doping	F. Huttmann, A. J. Martínez-Galera, V. Caciuc, N. Atodiresei, S. Schumacher, S. Standop, I. Hamada, T. O. Wehling, S. Blügel, T. Michely	Phys. Rev. Lett. 115, 236101	2015年12月	国外	○
5	Adsorption of reaction of H_2S on Cu(110) with scanning tunneling microscope	A. Shiotari, S. Hatta, H. Okuyama, T. Aruga, and I. Hamada	Phys. Chem. Chem. Phys. 18, 4541-4546	2016年1月	国外	○
6	First-Principles Study of Ion Diffusion in Perovskite Solar Cell Sensitizers	J. Haruyama, K. Sodeyama, L. Han, Y. Tateyama	J. Am Chem. Soc., 137, 10048-10051	2015年8月	国外	○
7	Surface Properties of CH3NH3PbI3 for Perovskite Solar Cell	J. Haruyama, K. Sodeyama, L. Han, Y. Tateyama	Acc. Chem. Res., 49, 554-556	2016年2月	国外	○
8	Corrosion Prevention Mechanism of Aluminum Metal in Superconcentrated Electrolytes	Yuki Yamada, Ching Hua Chiang, Keitaro Sodeyama, Jianhui Wang, Yoshitaka Tateyama, Atsuo Yamada	ChemElectroChem 2, 1687-1694	2015年7月	国外	○
9	A method to calculate redox potentials relative to the normal hydrogen electrode in nonaqueous solution by using density functional theory-based	Ryota Jono, Yoshitaka Tateyama, Koichi Yamashita	Phys. Chem. Chem. Phys. 17, 27103	2015年9月	国外	○
10	Near-Shore Aggregation Mechanism of Electrolyte Decomposition Products to Explain Solid Electrolyte Interphase Formation	Keisuke Ushirogata, Keitaro Sodeyama, Zdenek Futera, Yoshitaka Tateyama, Yukihiro Okuno	J. Electrochem. Soc. 162, A2670-A2678	2015年10月	国外	○
11	Investigating crystalline-polarity-dependent electronic structures of GaN by hard x-ray photoemission and ab-initio calculations	Takeo Ohsawa, Shigenori Ueda, Motohiro Suzuki, Yoshitaka Tateyama, Jesse R. Williams, Naoki Ohashi	Appl. Phys. Lett. 107, 171604	2015年10月	国外	○
12	Conservation of the pure adiabatic state in Ehrenfest dynamics of the photoisomerization of molecules	Yoshiyuki Miyamoto, Yoshitaka Tateyama, Norihisa Oyama, Takahisa Ohno	Sci. Rep. 5, 18220	2015年12月	国外	○
13	First-principles study on the cosensitization effects of Ru and squaraine dyes on a TiO_2 surface	Yusuke Ootani, Keitaro Sodeyama, Liyuan Han, Yoshitaka Tateyama	Surf. Sci. 649, 66-71	2016年2月	国外	○
14	Sodium-Ion Intercalation Mechanism in MXene Nanosheets	Satoshi Kajiyama, Lucie Szabova, Keitaro Sodeyama, Hiroki Iinuma, Ryohei Morita, Kazuma Gotoh, Yoshitaka Tateyama, Masashi Okubo, Atsuo Yamada	ACS Nano 10, 3334-3341	2016年2月	国外	○

15	Life of superoxide in aprotic Li-O_2 battery electrolytes: simulated solvent and counter-ion effects	Johan Scheers, D. Lidberg, Keitaro Sodeyama, Zdenek Futera, Yoshitaka Tateyama	Phys. Chem. Chem. Phys. 18, 9961-9968	2016年2月	国外	○
16	A Study on Electrolytic Corrosion of Boron-Doped Diamond Electrodes when Decomposing Organic Compounds	Takeshi Kashiwada, Takeshi Watanabe, Yusuke Ootani, Yoshitaka Tateyama, Yasuaki Einaga	ACS Appl. Mater. Interfaces	2016年3月	国外	○
17	Decomposition of the fluoroethylene carbonate additive and the glue effect of lithium fluoride products for the solid electrolyte interphase: an ab initio study	Yukihiro Okuno, Keisuke Ushirogata, Keitaro Sodeyama, Yoshitaka Tateyama	Phys. Chem. Chem. Phys. 18, 8643-8653	2016年3月	国外	○
18	Improving DIIS convergence for metallic systems using Gaussian basis set	David Sulzer, Satoru Iuchi, Koji Yasuda	Chemical Physics Letters 635 (2015) pp. 201-204	2015年7月	国外	○
19	Molecular dynamics study of the structure of anionic SDS, cationic DTAC, zwitterionic DDAO, and nonionic C12E8 spherical micelles in solution	Noriyuki Yoshii, Kazushi Fujimoto, Susumu Okazaki	J. Mol. Liq.	2015年12月	国外	○
20	Molecular dynamics study of the formation mechanisms of ionic SDS andnonionic C12E8 micelles and n-dodecane droplets	Shinji Kawada, Mika Komori, Kazushi Fujimoto, Noriyuki Yoshii, Susumu Okazaki	Chem. Phys. Lett.	2016年1月	国外	○
21	A molecular dynamics study of the breathing and deforming modes of the spherical ionic SDS and nonionic C12E8 micelles	Lin Wang, Kazushi Fujimoto, Noriyuki Yoshii, and Susumu Okazaki	J. Chem. Phys.	2016年1月	国外	○
22	Molecular dynamics study of lipid bilayers modeling the plasma membranes of mouse hepatocytes and hepatomas	Y Andoh, N Aoki, S Okazaki	J. Chem. Phys.	2016年2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	Mechanism of slow crystal growth of tetrahydrofuran clathrate hydrate	Takuma Yagasaki, Masakazu Matsumoto,Hideki Tanaka	J. Phys. Chem. C. 120, 3305−3313	2016年2月	国外	○
2	Anomalous thermodynamic properties of Ice XVI and metastable hydrates	Takuma Yagasaki, Masakazu Matsumoto,Hideki Tanaka	Phys. Rev. B 93, 054118	2016年2月	国外	○
3	Platinum-catalyzed reduction of amides with hydrosilanes bearing dual Si-H groups: a theoretical study of the reaction mechanism	N. Nakatani, J.-y. Hasegawa, Y. Sunada, and H. Nagashima	Dalton Transactions, 44, 19344-19356 (2015)	2015年10月	国外	○

4	Kinetic Analysis for the Multistep Profiles of Organic Reactions: Significance of the Conformational Entropy on the Rate Constants of the Claisen Rearrangement	Y. Sumiya, Y. Nagahata, T. Komatsuzaki, T. Taketsugu, and S. Maeda	J. Phys. Chem. A, 119, 11641-11649 (2015)	2015年11月	国外	○
5	Gold Nanoparticle Decoration of Insulating Boron Nitride Nanosheet on Inert Gold Electrode Towards an Efficient Electrocatalyst for the Reduction of Oxygen to Water	G. Elumalai, H. Noguchi, A. Lyalin, T. Taketsugu, and K. Uosaki	Electrochemistry Communications, 66 53-57 (2016)	2016年3月	国外	○
6	Long Range Functionalization of h-BN Monolayer by Carbon Doping	M. Gao, M. Adachi, A. Lyalin, and T. Taketsugu	J. Phys. Chem. C, in press http://doi.org/10.1021/acs.jpcc.5b12706	2016年3月	国外	○
7	Revisiting the extrapolation of correlation energies to complete basis set limit	Masaki Okoshi, Teruo Atsumi, Hiromi Nakai	J. Comput. Chem. 36, 1075 (2015)	2015年4月	国外	○
8	A divide-and-conquer method with approximate Fermi levels for parallel computations	Takeshi Yoshikawa, Hiromi Nakai	Theor. Chem. Acc. 134, 53 (2015)	2015年4月	国外	○
9	Accompanying coordinate expansion and recurrence relation method using a transfer relation scheme for electron repulsion integrals with high angular momenta and long contractions	Masao Hayami, Junji Seino, Hiromi Nakai	J. Chem. Phys. 142, 204110 (2015)	2015年5月	国外	○
10	Theoretical Analysis of the Oxidation Potentials of Organic Electrolyte Solvents	Masaki Okoshi, Atsushi Ishikawa, Yoshiumi Kawamura, Hiromi Nakai	ECS Electrochem. Lett. 4, A103 (2015).	2015年7月	国外	○
11	Theoretical Study of Extremely Long yet Stable Carbon-Carbon Bonds: Effect of Attractive C···H Interactions and Small Radical Stabilization of Diamondoids	Daeheum Cho, Yasuhiro Ikabata, Takeshi Yoshikawa, Jin Yong Lee, Hiromi Nakai	Bull. Chem. Soc. Jpn. 88, 1636 (2015)	2015年9月	国外	○
12	分割統治型密度汎関数強束縛分子動力学(DC-DFTB-MD)法の最近の展開	西村好史、海寶丈彰、中井浩巳	J. Comput. Chem. Jpn. 14, 43 (2015)	2015年9月	国内	○
13	Divide-and-Conquer-Type Density-Functional Tight-Binding Molecular Dynamics Simulations of Proton Diffusion in a Bulk Water System	Hiromi Nakai, Aditya Wibawa Sakti, Yoshifumi Nishimura	J. Phys. Chem. B 120, 217 (2016)	2015年12月	国外	○
14	Efficient two-component relativistic method for large systems	Hiromi Nakai	AIP Conf. Proc. 1702, 090030 (2015)	2015年12月	国外	○
15	Contrasting mechanisms for CO_2 absorption and regeneration processes in aqueous amine solutions: Insights from density-functional tight-binding molecular dynamics simulations	Hiromi Nakai, Yoshifumi Nishimura, Takeaki Kaiho, Takahito Kubota, Hiroshi Sato	Chem. Phys. Lett. 647, 127 (2016)	2016年1月	国外	○
16	Quantum chemical approach for condensed-phase thermochemistry (III): Accurate evaluation of proton hydration energy and standard hydrogen electrode potential	Atsushi Ishikawa, Hiromi Nakai	Chem. Phys. Lett. 650, 159 (2016)	2016年3月	国外	○
17	How Can We Understand Au8 Cores and Entangled Ligands of Selenolate- and Thiolate-protected Gold Nanoclusters Au24(ER)20 and Au20(ER)16 (E = Se, S; R = Ph, Me)? A Theoretical Study	N. Takagi, K. Ishimura, M. Matsui, R. Fukuda, T. Matsui, T. Nakajima, M. Ehara, S. Sakaki	J. Am. Chem. Soc. 137, 8593-8602 (2015).	2015年6月	国外	○