サブ課題Ａ：新エネルギー源の創出・確保ー太陽光エネルギー

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・雑誌等名）	発表した時期	国内・外の別	査読（有り）
1	Orbital-invariant spin-extended approximate coupled-cluster for multi-reference systems	土持崇嗣、天能精一郎	J. Chem. Phys., **149** 044109 (2018)	2018年7月	国外	有
2	Full coupled-cluster reduction for accurate description of strong electron correlation	許恩華、上島基之、天能精一郎	Phys. Rev. Lett., **121** 113001 (2018)	2018年9月	国外	有
3	Monte Carlo explicitly correlated many-body Green’s function theory	C. M. Johnson, A. E. Doran, 天能精一郎、 S. Hirata	J. Chem. Phys., **149** 174112 (2018)	2018年11月	国外	有
4	Extending spin-symmetry projected coupled-cluster to large model spaces using an iterative null-space projection technique	土持崇嗣、天能精一郎	J. Comput. Chem., **40** 267-280 (2019)	2018年12月	国外	有
5	Massively parallel sparse matrix function calculations with NTPoly	W. Dawson, T. Nakajima	Comput. Phys. Commun. **225**, 154-165 (2018). 10.1016/j.cpc.2017.12.010	2018年4月	国外	有
6	Theoretical study on mesoscopic-size impurity effects in the charge separation process of organic photocells	T. Shimazaki, M. Tashiro, T. Nakajima	Phys. Chem. Chem. Phys. **20**, 14846-14854 (2018). 10.1039/c7cp08125a	2018年5月	国外	有
7	High-throughput screening of perovskite oxynitride and oxide materials for visible-light photocatalysis	K. Sawada, T. Nakajima	APL Mater. **6**, 101103 (2018). 10.1063/1.5041784	2018年10月	国外	有
8	Antisymmetrized geminal powers with larger chemical basis sets	W. Uemura, T. Nakajima	Phys. Rev. A **99**, 012519 (2019). 10.1103/PhysRevA.99.012519	2019年1月	国外	有

9	A simple model for relative energies of all fullerenes reveals the interplay between intrinsic resonance and structural deformation effects in medium-sized fullerenes	B. Chan, Y. Kawashima, W. Dawson, M. Katouda, T. Nakajima, K. Hirao	J. Chem. Theory Comput. **15**, 1255-1264 (2019). 10.1021/acs.jctc.8b00981	2019年1月	国外	有
10	Investigations on the charge transfer mechanism at donor/acceptor interfaces in the quest for descriptors of organic solar cell performance	Azusa Muraoka, Mikiya Fujii, Kenji Mishima, Hiroki Matsunaga, Hiroaki Benten, Hideo Ohkita, Shinzaburo Ito, Koichi Yamashita	Phys. Chem. Chem. Phys., **20**, 12193 (2018)	2018年4月	国外	有
11	Two-dimensional optical excitations in mixed valence Cs2Au2I6 fully inorganic double perovskite	Giacomo Giorgi, Koichi Yamashita and Maurizia Palummo	J. Mater. Chem. C, **6**, 10197-10201 (2018)	2018年9月	国外	有
12	Nature of the Electronic and Optical Excitations of Ruddlesden-Popper Hybrid Organic-Inorganic Perovskites: The Role of the Many-Body Interactions	Giacomo Giorgi, Koichi Yamashita and Maurizia Palummo	J. Phys. Chem. Lett., **9**, 5891-5896 (2018)	2018年9月	国外	有
13	Molecular QTAIM Topology Is Sensitive to Relativistic Corrections	James S. M. Anderson, Juan I. Rodríguez, Paul W. Ayers, Daniel E. Trujillo-González; Andreas W. Goetz; Jochen Autschbach, F. L. Castillo-Alvarado, Koichi Yamashita	Chemistry: A European Journal, **25**, 2538-2544 (2019)	2019年1月	国外	有
14	Significance of hydrogen bonding and other noncovalent interactions in determining octahedral tilting in the CH3NH3PbI3 hybrid organic-inorganic halide perovskite solar cell semiconductor	Pradeep Varadwaj, Arpita Varadwaj, Helder M. Marques, and Koichi Yamashita	Scientific Reports, 9(1):50 (2019)	2019年1月	国外	有
15	Regression model for stabilization energies associated with anion ordering in perovskite-type oxynitrides	Masanori Kaneko, Mikiya Fujii, Takashi Hisatomi, Koichi Yamashita, Kazunari Domen	Journal of Energy Chemistry, **36**, 7-14 (2019)	2019年1月	国外	有

16	Effect of Nuclear Motion on Charge Transport in Fullerenes	Saeid Arabnejad, Amrita Pal, Koichi Yamashita, Sergei Manzhos	Frontiers in Energy Research, 7:3, 1-7 (2019)	2019年1月	国外	有
17	First-principles study on visible light absorption of defected SrNbO3	Masanori Kaneko, Kenji Mishima, Koichi Yamashita	J. Photochemistry & Photobiology A: Chemistry, **375**, 175-180 (2019)	2019年2月	国外	有
18	Simulation of Conductive Atomic Force Microscopy of Organic Photovoltaics by Dynamic Monte Carlo Method	Eisuke Kawashima, Mikiya Fujii, Koichi Yamashita	Chem. Lett. (doi:10.1246/cl.190041) (2019)	2019年3月	国内	有

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

2. 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・雑誌等名）	発表した時期	国内・外の別	査読（有り）
1	Hydrogen adsorption on Pt(111) revisited from random phase approximation	Lei Yan, Yang Sun, Yoshiyuki Yamamoto, Shusuke Kasamatsu, Ikutaro Hamada, and Osamu Sugino	Journal of Chemical Physics	2018年10月	国外	有
2	Direct coupling of first-principles calculations with replica exchange Monte Carlo sampling of ion disorder in solids	Shusuke Kasamatsu and Osamu Sugino	Journal of Physics: Condensed matter	2019年2月	国外	有
3	First-Principles Microkinetic Analysis of NO + CO Reactions on Rh(111) Surface toward Understanding NOx Reduction Pathways	Atsushi Ishikawa, Yoshitaka Tateyama	J. Phys. Chem. C **122**, 17378-17388	2018年7月	国外	有
4	Structures, Electronic States, and Reactions at Interfaces between LiNi0.5Mn1.5O4 Cathode and Ethylene Carbonate Electrolyte: A First-Principles Study	Yukihiro Okuno, Keisuke Ushirogata, Keitaro Sodeyama, Ganes Shukri, Yoshitaka Tateyama	J. Phys. Chem. C **123**, 2267-2277	2019年1月	国外	有

5	リチウムイオン電池 Solid Electrolyte Interphase (SEI) に関する第一原理計算研究	館山佳尚	J. Comput. Chem. Jpn. **18**, 18-28	2019年2月	国内	有
6	In Situ Spectroscopic Study on the Surface Hydroxylation of Diamond Electrodes	Seiji Kasahara, Taiga Ogose, Norihito Ikemiya, Takashi Yamamoto, Keisuke Natsui, Yasuyuki Yokota, Raymond A. Wong, Shota Iizuka, Nagahiro Hoshi, Yoshitaka Tateyama, Yousoo Kim, Masashi Nakamura, Yasuaki Einaga	Anal. Chem. **91**, 4980-4986	2019年3月	国外	有
7	Microscopic Elucidation of Solid-Electrolyte Interphase (SEI) Film Formation via Atomistic Reaction Simulations: Importance of Functional Groups of Electrolyte and Intact Additive Molecules	Norio Takenaka, Masataka Nagaoka	The Chemical Record, **19**, 1-13 (2019)	2019年3月	国外	有
8	The crucial role of electron transfer from interfacial molecules in the negative potential shift of Au electrode immersed in ionic liquids	T. Inagaki, N. Takenaka, and M. Nagaoka	Physical Chemistry Chemical Physics, **20**, 29362 (2018)	2018年10月	国外	有
9	Atomistic chemical computation of Olefin polymerization reaction catalyzed by (pyridylamido)hafnium(IV) complex: Application of Red Moon simulation	K. Matsumoto, M. Takayanagi, Y. Suzuki, N. Koga, and M. Nagaoka	Journal of Computational Chemistry, **40**, 421 (2019)	2018年10月	国外	有
10	Concentration Effect of Fluoroethylene Carbonate on the Formation of Solid Electrolyte Interphase Layer in Sodium-Ion Batteries	A. Bouibes, N. Takenaka, T. Fujie, K. Kubota, S. Komaba, and M. Nagaoka	ACS Applied Materials & Interfaces, **10**, 28525 (2018)	2018年8月	国外	有
11	Red Moon methodology compatible with quantum mechanics/molecular mechanics framework: Application to solid electrolyte interphase film formation in lithium-ion battery system	T. Fujie, N. Takenaka, Y. Suzuki, and M. Nagaoka	The Journal of Chemical Physics, **149**, 044113 (2018)	2018年7月	国外	有
12	Cost-Effective Method for Free-Energy Minimization in Complex Systems with Elaborated Ab Initio Potentials	C. Bistafa, Y. Kitamura, M. T. C. Martins-Costa, M. Nagaoka, and M. F. Ruiz-López	Journal of Chemical Theory and Computation, **14**, 3262, (2018)	2018年5月	国外	有

13	Exploring the effect of pendent side chain length on the structural and mechanical properties of hydrated perfluorosulfonic acid polymer membranes by molecular dynamics simulation	A.-T. Kuo, K. Takeuchi, A. Tanaka, S. Urata, S. Okazaki, W. Shinoda	Polymer, **146**, 53-62	2018年5月	国外	有
14	Difference in molecular mechanisms governing changes in membrane properties of phospholipid bilayers induced by addition of nonionic and zwitterionic surfactants	Y. Andoh, S. Kitou, S. Okazaki	J. Mol. Liquids, **271**, 933-941	2018年9月	国外	有
15	Molecular mechanism of material deformation and failure in butadiene rubber: Insight from all-atom molecular dynamics simulation using a bond breaking potential model	R. S. Payal, K. Fujimoto, C. Jang, W. Shinoda, Y. Takei, H. Shima, K. Tsunoda, S. Okazaki	Polymer, **170**, 113-119	2019年3月	国外	有
16	Development of dissociative force field for all-atomistic molecular dynamics calculation of fracture of polymers	K. Fujimoto, R. S. Payal, T. Hattori, W. Shinoda, M. Nakagaki, S. Sakaki, S. Okazaki	J. Comp. Chem. accepted.		国外	有

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

2. 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・雑誌等名）	発表した時期	国内・外の別	査読（有り）
1	Phase Diagrams of TIP4P/2005, SPC/E, and TIP5P Water at High Pressure	T. Yagasaki, M. Matsumoto, H. Tanaka	J. Phys. Chem. B **122**, 7718-7725 (2018).	2018年7月	国外	有
2	On the Phase Behaviors of Hydrocarbon and Noble Gas Clathrate Hydrates: Dissociation Pressures, Phase Diagram, Occupancies, and Equilibrium with Aqueous Solution	H. Tanaka, T. Yagasaki, M. Matsumoto	J. Chem. Phys. **149**, 074502, 1-15 (2018).	2018年8月	国外	有
3	Phase diagram of ice polymorphs under negative pressure considering the limits of mechanical stability	T. Matsui, T. Yagasaki, M. Matsumoto, H. Tanaka	J. Chem. Phys. **150**, 04102, 1-6 (2019).	2019年1月	国外	有

4	Molecular Dynamics Study of Kinetic Hydrate Inhibitors: The Optimal Inhibitor Size and Effect of Guest Species	T. Yagasaki, M. Matsumoto, H. Tanaka	J. Phys. Chem. C **123**, 1806-1816 (2019).	2019年1月	国外	有
5	Lithiation Products of a Silicon Anode Based on Soft X-ray Emission Spectroscopy: A Theoretical Study	A. Lyalin, V. G. Kuznetsov, A. Nakayama, I. V. Abarenkov, I. I. Tupitsyn, I. E. Gabis, K. Uosaki, and T. Taketsugu	J. Phys. Chem. C, **122**, 11096-11108 (2018).	2018年5月	国外	有
6	A First-Order Interacting Space Approach to Excited-State Molecular Interaction: Solvatochromic Shift of p-Coumaric Acid and Retinal Schiff Base	K. Yanai, K. Ishimura, A. Nakayama, and J. Hasegawa	J. Chem. Theory Comput., **14**, 3643 (2018).	2018年6月	国外	有
7	Defect-induced efficient dry reforming of methane over two-dimensional Ni/h-boron nitride nanosheet catalysts	Y. Cao, P. Maitarad, M. Gao, T. Taketsugu, H. Li, T. Yan, L. Shi, and D. Zhang	App. Catal. B: Environ., **238**, 51-60 (2018).	2018年7月	国外	有
8	Visualization of the Intrinsic Reaction Coordinate and Global Reaction Route Map by Classical Multidimensional Scaling	T. Tsutsumi, Y. Ono, Z. Arai, and T. Taketsugu	J. Chem. Theory Comput., **14**, 4263-4270 (2018).	2018年7月	国外	有
9	Microscopic Electrode Processes in the Four-Electron Oxygen Reduction on Highly Active Carbon-Based Electrocatalysts	K. Sakaushi, M. Eckardt, A. Lyalin, T. Taketsugu, R. J. Behm, and K. Uosaki	ACS Catalysis, **8**, 8162-8176 (2018).	2018年7月	国外	有
10	On-the-fly molecular dynamics study of the excited-state branching reaction of α-methyl-cis-stilbene	T. Tsutsumi, Y. Harabuchi, R. Yamamoto, S. Maeda, and T. Taketsugu	Chem. Phys., **515**, 564-571 (2018).	2018年8月	国外	有
11	Theoretical investigations on hydrogen peroxide decomposition in aquo	T. Tsuneda and T. Taketsugu	Phys. Chem. Chem. Phys., **20**, 24992-24999 (2018).	2018年9月	国外	有
12	Constraint Structure Optimization to a Specific Minimum Using Ionization Energy	I. Harada, A. Nakayama, J. Hasegawa	J. Comput. Chem., **40**, 507-514 (2019)	2018年10月	国外	有

13	Ab initio surface hopping excited-state molecular dynamics approach on the basis of spin-orbit coupled states: An application to the A-band photodissociation of CH3I	M. Kamiya and T. Taketsugu	J. Comput. Chem., **40**, 456-463 (2019).	2018年11月	国外	有
14	CO2 Adsorption on $Ti3O6^-$: A Novel Carbonate Binding Motif	S. Debnath, X. Song, M. Fagiani, M. Weichman, M. Gao, S. Maeda, T. Taketsugu, W. Schöllkopf, A. Lyalin, D. Neumark, and K. Asmis	J. Phys. Chem. C, **123**, 8439-8446 (2019).	2018年12月	国外	有
15	Combined Automated Reaction Pathway Searches and Sparse Modeling Analysis for Catalytic Properties of Lowest Energy Twins of Cu13	T. Iwasa, T. Sato, M. Takagi, M. Gao, A. Lyalin, M. Kobayashi, K. Shimizu, S. Maeda, and T. Taketsugu	J. Phys. Chem. A, **123**, 210-217 (2019).	2019年1月	国外	有
16	Soft X-ray Li-K and Si-L2,3 Emission from Crystalline and Amorphous Lithium Silicides in Lithium-ion Batteries Anode	A. Lyalin, V. G. Kuznetsov, A. Nakayama, I. V. Abarenkov, I. I. Tupitsyn, I. E. Gabis, K. Uosaki, and T. Taketsugu	J. Electrochem. Soc., **166**, A5362-A5368 (2019).	2019年1月	国外	有
17	The Role of Nitrogen-doping and the Effect of the pH on the Oxygen Reduction Reaction on Highly Active Nitrided Carbon Sphere Catalysts	M. Eckardt, K. Sakaushi, A. Lyalin, M. Wassner, N. Hüsing, T. Taketsugu, and R.J. Behm	Electrochimica Acta, **299**, 736-748 (2019).	2019年1月	国外	有
18	Ab initio surface hopping molecular dynamics on the dissociative recombination of CH3+	T. Taketsugu and Y. Kobayashi	Comp. Theo. Chem., **1150**, 1-9 (2019).	2019年1月	国外	有
19	Low-lying Excited States of hqxcH and Zn-hqxc Complex: Toward Understanding Intramolecular Proton Transfer Emission	M. Ebina, Y. Kondo, T. Iwasa, T. Taketsugu	Inorg. Chem., **58**, 4686-4698 (2019).	2019年3月	国外	有
20	Perspective on Density-Functional Tight-Binding Parameterization towards Transition Metals	周建斌、中井浩巳	分子シミュレーション研究会会誌アンサンブル 20, 8 (2018)	2018年1月	国内	有

21	分割統治型密度汎関数強束縛(DC-DFTB)法に対する最近の開発と応用	西村好史、中井浩巳	分子シミュレーション研究会会誌アンサンブル **20**, 18-23 (2018)	2018年1月	国内	有
22	光受容タンパク質の機構解明に向けた分割統治型時間依存密度汎関数強束縛法の開発	河本奈々、吉川武司、小野純一、中井浩巳	J. Comput. Chem. Jpn **17**, 127 (2018)	2018年10月	国内	有
23	Development of Divide-and-Conquer Density-Functional Tight-Binding Method for Theoretical Research on Li-ion Battery	Chien-Pin Chou, Aditya Wibawa Sakti, Yoshifumi Nishimura, Hiromi Nakai	Chem. Rec. **19**, 746-757 (2019).	2018年11月	国外	有
24	Development of Large-Scale Excited-State Calculations Based on the Divide-and-Conquer Time-Dependent Density Functional Tight-Binding Method	Nana Komoto, Takeshi Yoshikawa, Junichi Ono, Yoshifumi Nishimura, Hiromi Nakai	J. Chem. Theory Comput. **15**, 1719-1727 (2019)	2019年1月	国外	有
25	DCDFTBMD: Divide-and-Conquer Density Functional Tight-Binding Program for Huge-System Quantum Mechanical Molecular Dynamics Simulations	Yoshifumi Nishimura, Hiromi Nakai	J. Comput. Chem. **40**, 1538-1549 (2019)	2019年3月	国外	有
26	DCDFTBMDプログラムの公開	西村好史、吉川武司、中井浩巳	J. Comput. Chem. Jpn **17**, A21 (2018)	2019年3月	国内	有