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. W ójcik, 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	○