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