

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      | ○             |

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| 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 | ○ |