様式－ 2

研究業績等

氏名　塩田　淑仁

平成30年3月27日現在

区分	番号	事項
【原著論文】	1	Yoshizawa, K.; Yokomichi, Y.; **Shiota, Y.**; Ohta, T.; Yamabe, T. “Density functional study on possible peroxo form of non-heme diiron enzyme model,” *Chem. Lett.,* **1997**, 587-588.
	2	Yoshizawa, K.; Ohta, T.; **Shiota, Y**.; Yamabe, T. “Cleavage of C-H Bond of Methane on Intermediate Q of Methane Monooxygenase,” *Chem. Lett.,* **1997**, 1213-1214.
	3	Yamabe, T.; Nakamura, K.; **Shiota, Y**.; Yoshizawa, K.; Kawauchi, S.; Ishikawa, M. “Novel Aspects of the [1,3] Sigmatropic Silyl Shift in Allylsilane,” *J. Am. Chem. Soc.,* **1997**, *119*, 807-815.
	4	Yoshizawa, K.; **Shiota, Y.**; Yamabe, T. “Reaction paths for the conversion of methane to methanol catalyzed by FeO^+,” *Chem. Eur. J.,* **1997**, *3*, 1160-1169.
	5	Takeuchi, T.; Yoshizawa, K.; **Shiota, Y.**; Nakamura, O.; Kageyama, H.; Yamabe, T. “Orbital interaction and vibrational mode analyses for phase transitions of $BaTiO_3$,” *J. mater. chem.,* **1997**, *7*, 969-975.
	6	Yoshizawa, K.; **Shiota, Y.**; Kang, S.; Yamabe, T. “Possible nitrogen fixation by disilabutadiene,” *Organometallics*, **1997**, *16*, 5058-5063.
	7	Yoshizawa, K.; **Shiota, Y.**; Yamabe, T. “Methane-methanol conversion by MnO^+, FeO^+, and CoO^+: A theoretical study of catalytic selectivity,” *J. Am. Chem. Soc.,* **1998**, *120*, 564-572.
	8	Yoshizawa, K.; **Shiota, Y.**; Yamabe, T. “Abstraction of the hydrogen atom of methane by iron-oxo species: The concerted reaction path is energetically more favorable,” *Organometallics,* **1998**, *17*, 2825-2831.
	9	Yoshizawa, K.; **Shiota, Y.**; Yamabe, T. “Intrinsic reaction coordinate analysis of the conversion of methane to methanol by an iron-oxo species: A study of crossing seams of potential energy surfaces,” *J. Chem. Phys.,* **1999**, *111*, 538-545.
	10	Yoshizawa, K.; **Shiota, Y.**; Yamabe, T. “Reaction pathway for the direct benzene hydroxylation by iron-oxo species,” *J. Am. Chem. Soc.,* **1999**, *121*, 147-153.
	11	Yoshizawa, K.; **Shiota, Y.**; Yumura, T.; Yamabe, T. “Direct Methane-Methanol and Benzene-Phenol Conversions on Fe-ZSM-5 Zeolite: Theoretical Predictions on the Reaction Pathways and Energetics,” *J. Phys. Chem. B,* **2000**, *104*, 734-740.
	12	Yoshizawa, K.; Kagawa, Y.; **Shiota, Y.** “Kinetic isotope effects in a C-H bond dissociation by the iron-oxo species of cytochrome P450,” *J. Phys. Chem. B,* **2000**, *104*, 12365-12370.
	13	Yoshizawa, K.; **Shiota, Y.**; Kagawa, Y.; Yamabe, T. “Femtosecond Dynamics of the Methane - Methanol and Benzene - Phenol Conversions by an Iron - Oxo Species,” *J. Phys. Chem. A* **2000**, *104*, 2552-2561.
	14	**Shiota, Y.**; Yoshizawa, K.; Ymabe, T. “Methane-to-methanol conversion by first-row transition-metal oxide ions: ScO^+, TiO^+, VO^+, CrO^+, MnO^+, FeO^+, CoO^+, NiO^+, and CuO^+,” *J. Am. Chem.,* **2000**, *122*, 12317-12326.
	15	Yoshizawa, K.; Suzuki, A.; **Shiota, Y**.; Yamabe, T. “Conversion of methane to methanol on diiron and dicopper enzyme models of methane monooxygenase: A theoretical study on a concerted reaction pathway,” *Bull. Chem. Soc. Jpn.,* **2000**, *73*, 815.
	16	Yoshizawa, K.; Yumura, T.; **Shiota, Y.**; Yamabe, T. “Formation of an iron-oxo species upon decomposition of dinitrogen oxide on a model of Fe-ZSM-5 zeolite,” *Bull. Chem. Soc. Jpn.,* **2000**, *73*, 29-36.
	17	Yoshizawa, K.; **Shiota, Y.**; Kagawa, Y. “Energetics for the oxygen rebound mechanism of alkane hydroxylation by the iron-oxo species of cytochrome P450,” *Bull. Chem. Soc. Jpn.,* **2000**, *73*, 2669-2673.
	18	Yoshizawa, K.; Kamachi, T.; **Shiota, Y**. “A theoretical study of the dynamic behavior of alkane hydroxylation by a compound I model of cytochrome P450,” *J. Am. Chem. Soc.* **2001**, *123*, 9806-9816.
	19	Ohta, T.; Kamachi, T.; **Shiota, Y.**; Yoshizawa, K. “A theoretical study of alcohol oxidation by ferrate,” *J. Org. Chem.* **2001**, *66*, 4122-4131.
	20	Yumura, T.; **Shiota, Y**.; Yoshizawa, K. “Reaction Pathways for the He, Li, and Li^+ Penetrations of the Benzene Ring,” *JCPE Journal,* **2001**, *13*, 169-176.

（注）用紙が不足する場合は，この様式をコピーしてください

様式− 2

研究業績等

氏名　塩田　淑仁

平成30年3月27日現在

区分	番号	事項
【原著論文】	21	**Shiota, Y.**; Kondo, M.; Yoshizawa, K. “Role of molecular distortions in the spin-orbit coupling between the singlet and triplet states of the 4π electron systems C_4H_4, $C_5H_5^+$, and $C_3H_3^-$,” *J. Chem. Phys.* **2001**, *115*, 9243-9254.
	22	Kondo, M.; **Shiota, Y.**; Yoshizawa, K. “Possible photoinduced spin transitions in bis(phenylmethylenyl)[2.2]paracyclophanes. A spin-orbit coupling study,” *J. Phys. Chem. A* **2002**, *106*, 7915-7920.
	23	**Shiota, Y.**; Yoshizawa, K. “A spin-orbit coupling study on the spin inversion processes in the direct methane-to-methanol conversion by FeO^+,” *J. Chem. Phys.* **2003**, *118*, 5872-5879.
	24	Kamachi, T.; **Shiota, Y**.; Ohta, T.; Yoshizawa, K. “Does the hydroperoxo species of cytochrome P450 participate in olefin epoxidation with the main oxidant, compound I? Criticism from density functional theory calculations,” *Bull. Chem. Soc. Jpn.,* **2003**, *76*, 721-732.
	25	Yoshizawa, K.; **Shiota, Y.**; Kamachi, T. “Mechanistic proposals for direct benzene hydroxylation over Fe-ZSM-5 zeolite,” *J. Phys. Chem. B* **2003**, *107*, 11404-11410.
	26	**Shiota, Y.**; Kihara, N.; Kamachi, T.; Yoshizawa, K. “A theoretical study of reactivity and regioselectivity in the hydroxylation of adamantane by ferrate(VI),” *J. Org. Chem.* **2003**, *68*, 3958-3965.
	27	**Shiota, Y.**; Yoshizawa, K. “QM/MM study of the mononuclear non-heme iron active site of phenylalanine hydroxylase,” *J Phys. Chem. B* **2004**, *108*, 17226-17237.
	28	Naka, A.; Ohnishi, H.; Miyahara, I.; Hirotsu, K.; **Shiota, Y.**; Yoshizawa, K.; Ishikawa, M. “Silicon-carbon unsaturated compounds. 69, Reactions of silenes produced thermally from pivaloyl- and adamantoyltris (trimethylsilyl) silane with silyl-substituted butadiynes and enynes,” *Organometallics,* **2004**, *23*, 4277-4287.
	29	**Shiota, Y.**; Yasunaga, M.; Naka, A.; Ishikawa, M.; Yoshizawa, K. “Theoretical study of thermal isomerization of silacyclobutene to cyclopropene,” *Organometallics,* **2004**, *23*, 4744-4749.
	30	**Shiota, Y.**; Suzuki, K.; Yoshizawa, K. “Mechanism for the direct oxidation of benzene to phenol by FeO^+,” *Organometallics,* **2005**, *24*, 3532-3538.
	31	Kamachi, T.; Kihara, N.; **Shiota, Y**.; Yoshizawa, K. “Computational exploration of the catalytic mechanism of dopamine β-monooxygenase: Modeling of its mononuclear copper active sites”, *Inorg. Chem.* **2005**, *44*, 4226-4236.
	32	Kojima, T.; Hayashi, K.-I.; **Shiota, Y**.; Tachi, Y.; Naruta, Y.; Suzuki, T.; Uezu, K.; Yoshizawa, K. “Synthesis and characterization of ruthenium(II)-nitrile complexes with bisamide-tpa ligands (tpa = tris(2-pyridylmethyl)amine),” *Bull. Chem. Soc. Jpn.,* **2005**, *78*, 2152-2158.
	33	**Shiota, Y.**; Suzuki, K.; Yoshizawa, K. “QM/MM Study on the Catalytic Mechanism of Benzene Hydroxylation over Fe-ZSM-5,” *Organometallics* **2006**, *25*, 3118-3123.
	34	Yoshizawa, K.; **Shiota, Y**. “Conversion of methane to methanol at the mononuclear and dinuclear copper sites of particulate methane monooxygenase (pMMO): A DFT and QM/MM study,” *J. Am. Chem. Soc.* **2006**, *128*, 9873-9881.
	35	Yoshizawa, K.; Kihara, N.; **Shiota, Y**.; Seino, H.; Mizobe, Y. “DFT calculations of cubane-type $Mo_2Ru_2S_4$ clusters. Stability of a possible dinitrogen cluster and an isolable acetonitrile cluster,” *Bull. Chem. Soc. Jpn.,* **2006**, *79*, 53-58.
	36	Yoshizawa, K.; Kihara, N.; Kamachi, T.; **Shiota, Y**. “Catalytic mechanism of dopamine β-monooxygenase mediated by Cu(III)-oxo,” *Inorg. Chem.* **2006**, *45*, 3034-3041.
	37	Kozlowski, P. M.; **Shiota, Y**.; Gomita, S.; Seino, H.; Mizobe, Y.; Yoshizawa, K. “DFT analysis of cubane-type $FeIr_3S_4$ clusters. Dinitrogen binding and activation at the tetrahedral Fe site,” *Bull. Chem. Soc. Jpn.,* **2007**, *80*, 2323-2328.
	38	Ito, Y.; Kondo, H.; **Shiota, Y.**; Yoshizawa, K. “Theoretical analysis of the reaction mechanism of biotin carboxylase,” *J. Chem. Theory Comput.* **2008**, *4*, 366-374.
	39	Hirai, Y.; Kojima, T.; Mizutani, Y.; **Shiota, Y.**; Yoshizawa, K.; Fukuzumi, S. “Ruthenium-catalyzed selective and efficient oxygenation of hydrocarbons with water as an oxygen source,” *Angew Chem. Int. Ed.* **2008**, *47*, 5772-5776.

（注）用紙が不足する場合は，この様式をコピーしてください

様式－ 2

研究業績等

氏名　塩田　淑仁

平成30年3月27日現在

区分	番号	事項
【原著論文】	40	Kojima, T.; Noguchi, D.; Nakayama, T.; Inagaki, Y.; **Shiota, Y.**; Yoshizawa, K.; Ohkubo, K.; Fukuzumi, S. "Synthesis and characterization of novel ferrocene-containing pyridylamine ligands and their ruthenium(II) complexes: Electronic communication through hydrogen-bonded amide linkage," *Inorg. Chem.* **2008**, *47*, 886-895.
	41	Inoue, T.; **Shiota, Y.**; Yoshizawa, K. "Quantum chemical approach to the mechanism for the biological conversion of tyrosine to dopaquinone," *J Am. Chem. Soc.* **2008**, *130*, 16890-16897.
	42	Tanaka, H.; **Shiota, Y.**; Matsuo, T.; Kawaguchi, H.; Yoshizawa, K. "DFT study on N_2 activation by a hydride-bridged diniobium complex. N≡N Bond cleavage accompanied by H_2 evolution," *Inorg. Chem.* **2009**, *48*, 3875-3881.
	43	Li, J.; **Shiota, Y.**; Yoshizawa, K. "Metal-ligand cooperation in H_2 production and H_2O decomposition on a Ru(II) PNN complex: The role of ligand dearomatization-aromatization," *J. Am. Chem. Soc.* **2009**, *131*, 13584-13585.
	44	**Shiota, Y.**; Yoshizawa, K. "Comparison of the reactivity of bis(μ-oxo)$Cu^{II}Cu^{III}$ and $Cu^{III}Cu^{III}$ species to methane," *Inorg Chem.* **2009**, *48*, 838-845.
	45	Tsutsumi, H.; Sunada, Y.; **Shiota, Y.**; Yoshizawa, K.; Nagashima, H. "Nickel(II), Palladium(II), and Platinum(II) η^3-Allyl Complexes Bearing a Bidentate Titanium(IV) Phosphinoamide Ligand: A Ti←M2 Dative Bond Enhances the Electrophilieity of the π-Allyl," *Organometallics,* **2009**, *28*, 1988-1991.
	46	**Shiota, Y.**; Sato, D.; Juhász, G.; Yoshizawa, K. "Theoretical study of thermal spin transition between the singlet state and the quintet state in the $[Fe(2\text{-picolylamine})3]^{2+}$ spin crossover system," *J. Phys. Chem. A* **2010**, *114*, 5862-5869.
	47	Kojima, T.; Hirasa, N.; Noguchi, D.; Ishizuka, T.; Miyazaki, S.; **Shiota, Y.**; Yoshizawa, K.; Fukuzumi, S. "Synthesis and characterization of ruthenium(II)-pyridylamine complexes with catechol pendants as metal binding sites," *Inorg. Chem.* **2010**, *49*, 3737-3745.
	48	Kojima, T.; Hirai, Y.; Ishizuka, T.; **Shiota, Y.**; Yoshizawa, K.; Ikemura, K.; Ogura, T.; Fukuzumi, S. "A low-spin ruthenium(IV)-oxo complex: Does the spin state have an impact on the reactivity?," *Angew. Che. Int. Ed.* **2010**, *49*, 8449-8453.
	49	Sato, D.; **Shiota, Y.**; Juhász, G.; Yoshizawa, K. "Theoretical study of the mechanism of valence tautomerism in cobalt complexes," *J. Phys. Chem. A,* **2010**, *114*, 12928-12935.
	50	Ishizuka, T.; Sawaki, T.; Miyazaki, S.; Kawano, M.; **Shiota, Y.**; Yoshizawa, K.; Fukuzumi, S.; Kojima, T. "Mechanistic insights into photochromic behavior of a ruthenium(II)- Pterin complex," *Chem. Eur. J.* **2011**, *17*, 6652-6662.
	51	Ishizuka, T.; Tobita, K.; Yano, Y.; **Shiota, Y.**; Yoshizawa, K.; Fukuzumi, S.; Kojima, T. "Proton-Coupled Electron Shuttling in a Covalently Linked Ruthenium-Copper Heterodinuclear Complex," *J. Am. Chem. Soc.* **2011**, *133*, 18570-18573.
	52	Tanaka, H.; Kondo, Y.; **Shiota, Y.**; Naka, A.; Ishikawa, M.; Yoshizawa, K. "Theoretical study on the formation of silacyclopropene from acylsilane and acetylene via silene-to-silylene rearrangement," *Organometallics,* **2011**, *30*, 3160-3167.
	53	**Shiota, Y.**; Herrera, J. M.; Juhász, G.; Abe, T.; Ohzu, S.; Ishizuka, T.; Kojima, T.; Yoshizawa, K. "Theoretical study of oxidation of cyclohexane diol to adipic anhydride by $[Ru(IV)(O)(tpa)(H_2O)]^{2+}$ complex (tpa = tris(2-pyridylmethyl)amine)," *Inorg. Chem.* **2011**, *50*, 6200-6209.
	54	Liu, T.; Dong, D.-P.; Kanegawa, S.; Kang, S.; Sato, O.; **Shiota, Y.**; Yoshizawa, K.; Hayami, S.; Wu, S.; He, C.; Duan, C.-Y. "Reversible Electron Transfer in a Linear {Fe_2 Co} Trinuclear Complex Induced by Thermal Treatment and Photoirraditaion," *Angew. Chem. Int. Ed.,* **2012**, *51*, 4367-4370.
	55	Tanaka, H.; **Shiota, Y.**; Hori, K.; Naka, A.; Ishikawa, M.; Yoshizawa, K. "Substituent effects in thermal reactions of a silene with silyl-substituted alkynes: A theoretical study," *Organometallics*, **2012**, *31*, 4737-4747.
	56	Huang, S.-P.; **Shiota, Y.**; Yoshizawa, K. "DFT Study of the Mechanism for Methane Hydroxylation by Soluble Methane Monooxygenase (sMMO): Effects of Oxidation State, Spin State, and Coordination Number," *Dalton Tran.*, **2013**, *42*, 1011-1023.

（注）用紙が不足する場合は，この様式をコピーしてください

様式－ 2

研究業績等

氏名　塩田　淑仁

平成30年3月27日現在

区分	番号	事項
【原著論文】	57	Fukazawa, A.; Oshima, H.; **Shiota, Y.**; Takahashi, S.; Yoshizawa, K.; Yamaguchi, S. "Thiophene-Fused Bisdehydro[12]annulene that Undergoes the [2+2] Alkyne Cycloaddition by Either Light or Heat," *J. Am. Chem. Soc.*, **2013**, *135*, 1731-1734.
	58	Mitome, H.; Ishizuka, T.; **Shiota, Y.**; Yoshizawa, K.; Kojima, T. "Heteronuclear $Ru^{II}Ag^{I}$ complexes having a pyrroloquinolinequinone derivative as a bridging ligand," *Inorg. Chem.*, **2013**, *52*, 2274-2276.
	59	Sawaki, T.; Ishizuka, T.; Kawano, M.; **Shiota, Y.**; Yoshizawa, Y.; Kojima T. "Complete Photochromic Structural Change of Ruthenium(II)-Diimine Complexes Based on the Control of the Excited States by Metallation," *Chem. Eur. J.*, **2013**, *19*, 8978-8990.
	60	Ishizuka, T.; Saegusa, Y.; **Shiota, Y.**; Ohtake, K.; Yoshizawa, K.; Kojima, T. "Multiply-Fused Porphyrins—Effects of Extended π-Conjugation on the Optical and Electrochemical Properties," *Chem. Comm.* **2013,** *49*, 5939-5941.
	61	**Shiota, Y.**; Juhász, G.; Yoshizawa, K. "Role of Tyrosine Residue in Methane Activation at the Dicopper Site of pMMO: A DFT Study," *Inorg. Chem.,* **2013,** *52,* 7907-7917.
	62	Huang, S.-P.; Zhang, Q.; **Shiota, Y.**; Nakagawa, T.; Kuwabara, H.; Yoshizawa, K.; Adachi, C. "Computational Prediction for Singlet- and Triplet-Transition Energies of Charge-Transfer Compounds," *J. Chem. Theory Comput.*, **2013**, *9*, 3872-3877.
	63	Li, Z.-Y.; Dai, J.-W.; **Shiota, Y.**; Yoshizawa, K.; Kanegawa, S.; Sato, O. "Multi-step spin crossover accompanied by symmetry breaking in an Fe^{III} complex: Crystallographic evidence and DFT studies," *Chem. Eur. J.*, **2013**, *19*, 12498-12952.
	64	Liu, T.; Zheng, H.; Kang, S.; **Shiota, Y.**; Hayami, S.; Mito, M.; Sato, O.; Yoshizawa, K.; Kanagawa, S.; Duan, C. "A light-induced spin crossover actuated single-chain magnet," *Nature Commun.* **2013**, *4*, 2826.
	65	P. K. Sajith; **Shiota, Y.**; Yoshizawa, K. "Role of acidic proton in the decomposition of NO over dimeric Cu(I) active sites in Cu-ZSM-5 catalyst: A QM/MM study," *ACS Catal.,* **2014**, *4*, 2075-2085.
	66	Ishizuka, T.; Ohzu, S. Kotani, H.; **Shiota, Y.**; Yoshizawa, K.; Kojima, T. "Hydrogen atom abstraction reactions independent of C-H bond dissociation energies of organic substrates in water: Significance of oxidant-substrate adduct formation", *Chem. Sci.,* **2014**, *5*, 1429-1436.
	67	Kodera, M.; Tsuji, T.; Yasunaga, T.; Kawahara, Y.; Hirano, T.; Hitomi Y.; Nomura, T.; Ogura, T.; Kobayashi, T.; P. K. Sajith, ; **Shiota, Y.**; Yoshizawa, K. "Roles of carboxylate donors in O-O bond scission of peroxodi-iron(iii) to high-spin oxodi-iron(iv) with a new carboxylate-containing dinucleating ligand," *Chem. Sci.,* **2014**, *5* 2282-2292.
	68	Kojima, T.: Kobayashi, R.; Ishizuka, T.; Yamakawa, S.; Kotani, H.; Nakanishi, T.; Ohkubo, K.; **Shiota, Y.**; Yoshizawa, K.; Fukuzumi, S. "Binding of Scandium Ions to Metalloporphyrin-Flavin Complexes for Long-Lived Charge Separation," *Chem. Eur. J.*, **2014**, *20*, 15518-15532.
	69	Yao, Z.-S.; Mito, M.; Kamachi, T.; **Shiota, Y.**; Yoshizawa, K.; Azuma, N.; Miyazaki, Y.; Takahashi, K.; Zhang, K.; Nakanishi, T.; Kang, S.; Kanegawa, S.; O. Sato "Molecular Motor-driven Abrupt Anisotropic Shape Change in a Single Crystal of a Ni Complex", *Nature Chem.*, **2014**, *6*, 1079-1083.
	70	Ohzu, S.; Ishizuka, T.; Kotani, H.; **Shiota, Y.**; Yoshizawa, K.; Kojima, T. "A Tetranuclear Ru(II) Complex with a Dinucleating Ligand Forming Multi-Mixed-Valence States", *Inorg. Chem.*, **2014**, *53*, 12677-12679.
	71	Zang, M.; Sonoda, T.; **Shiota, Y.**; Mishima, M.; Yanai, H.; Fujita, M.; Taguchi, T. "Gas-phase acidity of 1,1-bis(trifluoromethanesulfonyl)propane derivatives and related compounds: Experimental and theoretical studies," *J. Phys. Org. Chem.*, **2015**, *28,* 181-86.
	72	Kang, S.; Zheng, H.; Liu, T.; Hamachi, K.; Kanegawa, S.; Sugimoto, K.; **Shiota, Y.**; Hayami, S.; Mito, M.; Nakamura, T.; Baker, M. L.; Nojiri, H.; Yoshizawa, K.; C. Duan, C.; Sato, O. "A Ferromagnetically Coupled Fe42 Cyanide-Bridged Nanocage," *Nature Commun.,* **2015**, *6*, 5955/1-6. DOI:10.1038/ncomms6955
	73	Kotani, H.; Kaida, S.; Ishizuka, T.; Sakaguchi, M.; Ogura, T.; **Shiota, Y.**; Yoshizawa, K.; Kojima, T. "Formation and Characterization of a Reactive Chromium(V)-Oxo Complex: A Mechanistic Insight into Hydrogen-Atom Transfer Reactions" *Chem. Sci.*, **2015**, *6,* 945-955. DOI:10.1039/C4SC02285H

（注）用紙が不足する場合は，この様式をコピーしてください

研究業績等

氏名　塩田　淑仁

平成30年3月27日現在

区分	番号	事項
【原著論文】	74	Mitome, H.; Ishizuka, T. **Shiota, Y**.; Yoshizawa, K.; Kojima, T. “Controlling the Redox Properties of a Pyrroloquinolinequinone (PQQ) Derivative in a Ruthenium(II) Coordination Sphere,” *Dalton Trans*., **2015**, *44*, 3151-3158. DOI:10.1039/C4DT03358B
	75	**Shiota, Y.**; Takahashi, S.; Ohzu, S.; Ishizuka, T.; Kojima, T.; Yoshizawa, K. “ Mechanistic Study of Methanol Oxidation by Ru^{IV}–oxo complexes,” *J. Porphyrins Phthalocyanines*., **2015**, *19*, 417-426. DOI:10.1142/S1088424615500285
	76	Suzuki, T.; Tanaka, H.; **Shiota, Y.**; Sajith, P. K.; Arikawa, Y.; Yoshizawa, K. “Proton-Assisted Mechanism of NO Reduction on a Dinuclear Ruthenium Complex,” *Inorg. Chem.,* **2015**, *54*, 7181–7191. DOI: 10.1021/acs.inorgchem.5b00394
	77	Sugimoto, H; Mikami, A.; Kai, K.; Sajith, P. K.; **Shiota, Y.**; Yoshizawa, K.; Asano, K.; Suzuki, T. Itoh, S. “Cis -1,2-Aminohydroxylation of Alkenes Involving a Catalytic Cycle of Osmium(III) and Osmium(V) Centers: Os^{V}(O)(NHTs) Active Oxidant with a Macrocyclic Tetradentate Ligand,” *Inorg. Chem.,* **2015**, *54*, 7073–7082. DOI: 10.1021/acs.inorgchem.5b01083
	78	Kotani, H.; Sugiyama, T. Ishizuka, T.; **Shiota, Y.**; Yoshizawa, K.; Kojima, T. “Redox-Noninnocent Bhavior of Tris(2-pyridylmethyl)amine Bound to Lewis Acidic Rh(III) Ion Induced by C-H Deprotonation” *J. Am. Chem. Soc.,* **2015**, *137*, 11222-11225. DOI: 10.1021/jacs.5b06237
	79	Sunada, Y.; Ishida, S.; Hirakawa, F.; **Shiota, Y.**; Yoshizawa, K.; Kanegawa, S.; Sato, O.; Nagashima, H.; Iwamoto, T. “Persistent four-coordinate iron-centered radical stabilized by π-donation” *Chem. Sci*., **2015**, *6*, 191-198. DOI: 10.1039/C5SC02601F
	80	Su S.-Q.; Kamachi, T.; Yao, A.-S.; Huang, Y.-G.; **Shiota, Y**.; Yoshizawa, K.; Azuma, N.; Miyazaki, Y.; Nakano, M.; Maruta, G.; Takeda, S.; Kang, S.; Kanegawa, S.; Sato, O. “Assembling an alkyl rotor to access abrupt and reversible crystalline deformation of a cobalt(II) complex” *Nature Commun*. **2015**, *6*, 8810. DOI: 10.1038/ncomms9810
	81	Kang, S.; **Shiota, Y.**; Kariyazaki, A.; Kanegawa, S.; Yoshizawa, K.; Sato, O. “Heterometallic Fe^{III}/K coordination polymer with a wide thermal hysteretic spin transition around room temperature” *Chem. Eur. J*., **2016**, *22*, 532-538. DOI: 10.1002/chem.201503392
	82	Ishizuka, T.; Watanabe, A.; Kotani, H.; Hong, D.; Satonaka, K.; Wada, T.; **Shiota, Y**.; Yoshizawa, K.; Ohara, K.; Yamaguchi, K.; Kato, S.; Fukuzumi, S.; Kojima, T. “Homogeneous Photocatalytic Water Oxidation with a Dinuclear Co^{III}-Pyridylmethylamine Complex” *Inorg. Chem*. **2016**, *55*, 1154-1164. DOI: 10.1021/acs.inorgchem.5b02336
	83	Takahashi, K.; Kawamukai, K.; Okai, M.; Mochida, T.; Sakurai, T.; Ohta, H.; Yamamoto, T.; Einaga, Y.; **Shiota, Y**.; Yoshizawa, K. “A new family of anionic Fe^{III} spin crossover complexes featuring a weak-field N_2O_4 coordination octahedron.” *Chem. Eur. J*., **2016**, *22*, 1253-1257. DOI:10.1002/chem.201504883
	84	Yoshimoto, K.; Yatabe T.; Matsumoto, M.; Robertson, A.; Nakai, H.; Tanaka, H.; Kamachi, T.; **Shiota, Y**.; Yoshizawa, K.; Asazawa, K. Tanaka, H.; Ogo, S. “Synthesis and Structure of a Water-soluble μ-η^{1}:η^{1}-N_2 Dinuclear Ru^{II} Complex with a Polyamine Ligand” *Chem. Lett*. **2016**, *45*, 149-151. DOI:10.1246/cl.151004
	85	Itoyama, S.; Doitomi, K.; Kamachi, T.; **Shiota, Y.**; Yoshizawa, K. “Possible Peroxo State of the Dicopper Site of Particulate Methane Monooxygenase from Combined Quantum Mechanics and Molecular Mechanics Calculations” *Inorg. Chem*. **2016**, *55*, 2771-2775. DOI: 10.1021/acs.inorgchem.5b02603
	86	Kodera, M.; Ishiga, S.; Tsuji, T.; Sakurai, K.; Hitomi, Y.; **Shiota, Y.**; P. K. Sajith; Yoshizawa, K.; Mieda, K.; Ogura, T. “Formation and High Reactivity of the anti-Dioxo Form of High-Spin μ-Oxodioxodiiron(IV) as the Active Species That Cleaves Strong C-H Bonds” *Chem. Eur. J*. **2016**, *22*, 1-14. DOI: 10.1002/chem.201600048
	87	Fujita, Y.; Abe, M.; **Shiota, Y.**; Suzuki, T.; Yoshizawa, K. “Computational Study of Cyclobutane-1,3-diylidene Dicarbenes: Ground-State Spin Multiplicity and New Strategy Toward the Synthesis of Bicyclo[1.1.0]but-1(3)-enes” *Bull. Chem. Soc. Jpn*., **2016**, *89*, 770-778. DOI: 10.1246/bcsj.20160051

（注）用紙が不足する場合は，この様式をコピーしてください

研究業績等

氏名　塩田　淑仁

平成30年3月27日現在

区分	番号	事項
【原著論文】	88	Huang, Y.-G.; **Shiota, Y.**; Wu, M.-Y.; Su, S.-Q.; Yao, Z.-S.; Kang, S.; Kanegawa, S.; Li, G.-L.; Wu, S.-Q.; Kamachi, T.; Yoshizawa, K.; Ariga, K.; Hong, M.-C.; Sato, O. "Superior thermoelasticity and shape-memory nanopores in a porous supramolecular organic framework", *Nature Commun*. **2016**, *7*, 11564. DOI: 10.1038/ncomms11564
	89	Murata, S.; Takahashi, K.; Sakurai, T.; Ohta, H.; Yamamoto, T.; Einaga, Y.; **Shiota, Y.**; Yoshizawa. K. "The Role of Coulomb Interactions for Spin Crossover Behaviors and Crystal Structural Transformation in Novel Anionic Fe(III) Complexes from a π-Extended ONO Ligand" *Crystals* **2016**, *6*, 49. DOI:10.3390/cryst6050049
	90	Mitome, H.; Ishizuka, T.; Kotani, H.; **Shiota, Y.**; Yoshizawa, K.; Kojima, T. "Mechanistic Insights into C-H Oxidations by Ruthenium(III)-Pterin Complexes: Impact of Basicity of the Pterin Ligand and Electron Ac-ceptability of the Metal Center on the Transition States" *J. Am. Chem. Soc.,* **2016**, *138*, 9508-9520. DOI: 10.1021/jacs.6b03785
	91	Koide. T.; Takesue, M.; Murafuji, T.; Satomi, K.; Suzuki, Y.; Kawamata, J.; Terai, T.; Suzuki, M.; Yamada, H.; **Shiota, Y**.; Yoshizawa, K.; Tani F. "An Azulene-Fused Tetracene Diimide with a Small HOMO–LUMO Gap" *ChemPlusChem* **2016,** *81*, DOI: 10.1002/cplu.201600356
	92	Kato, S.-I; Kijima, T.; **Shiota, Y.**; Yoshihara, T.; Tobita, S.; Yoshizawa, K.; Nakamura, Y. "Push–Pull Fluorenones and Benzazulenequinones: Regioselective [4 + 2] and [2 + 2] Cycloadditions of Benzopentalenequinone Derivative and Alkynes Bearing an Aniline Moiety" *Tetrahedron Lett*. **2016**, 57, 4604-4607. DOI: 10.1016/j.tetlet.2016.09.002
	93	Shimoyama, Y.; Ishizuka, T.; Kotani, H.; **Shiota, Y.**; Yoshizawa, K.; Mieda, K.; Ogura, T.; Okajima, T.; Nozawa, S.; Kojima, T. "A Ruthenium(III)-Oxyl Complex Bearing Strong Radical Character", *Angew Chem. Int. Ed*. **2016**, *55,* 14041-14045. DOI: 10.1002/anie.201607861
	94	Kanegawa, S.; **Shiota, Y**.; Kang, S.; Takahashi , K.; Okajima, H.; Sakamoto, A.; Iwata, T.; Kandori, H.; Yoshizawa, K.; Sato, O. "Directional Electron Transfer in Crystals of [CrCo] Dinuclear Complexes Achieved by Chirality-assisted Preparative Method" *J. Am. Chem. Soc*. **2016**, *138*, 14170-14173. DOI: 10.1021/jacs.6b05089
	95	Huang, Y.-G.; **Shiota, Y**. ; Su, S.-Q.; Wu, S.-Q.; Yao, Z.-S.; Li, G.-L.; Kanegawa, S.; Kang, S.; Kamachi, T.; Yoshizawa, K.; Ariga, K.; Sato, O. "Thermally Induced Intra-Carboxyl Proton Shuttle in a Molecular Rack-and-Pinion Cascade Achieving Macroscopic Crystal Deformation" *Angew Chem. Int. Ed*. **2016**, *55,* 14628–14632. DOI: 10.1002/anie.201607886 (Research highlights, Nature Nanotechnology vol.11 Dec. 2016, 1001)
	96	Tahara, A.; Tanaka, H.; Sunada, Y.; **Shiota, Y**.; Yoshizawa, K.; Nagashima, H. "Theoretical Study of the Catalytic Hydrogenation of Alkenes by a Disilaferracyclic Complex: Can the Fe–Si σ-Bond-Assisted Activation of H–H Bonds Allow Development of a Catalysis of Iron?" *J. Org. Chem*., **2016**, *81,* 10900–10911. DOI: 10.1021/acs.joc.6b01961
	97	Mahyuddin, M.; Staykov, A.; **Shiota, Y**.; Yoshizawa, K. "Direct Conversion of Methane to Methanol by Metal-Exchanged ZSM-5 Zeolite (Metal = Fe, Co, Ni, and Cu)" *ACS Catal*., **2016**, *6*, 8321-8331. DOI: 10.1021/acscatal.6b01721
	98	Yao, Z.-S.; Wu, .S.-Q.;Kitagawa, Y.; Su, S.-Q.; Huang, Y.-G.; Li, G.-L.; Ni, Z.-H.; Nojiri, H.; **Shiota, Y**.; Yoshizawa, K.; Kang, S.; Kanegawa, S.; Sato, O."Anisotropic Change in Magnetic Susceptibility of a Dynamic Single Crystal of Cobalt(II) Complex" , *Angew Chem. Int. Ed*. **2017** , *56*, 717-721. DOI: 10.1002/anie.201606165
	99	Suzuki, W.; Kotani, H.; Ishizuka, T.; Ohkubo, K.; **Shiota, Y.**; Yoshizawa, K.; Fukuzumi, S.; Kojima, T. "Thermodynamics and Photodynamics of a Monoprotonated Porphyrin Directly Stabilized by Hydrogen Bonding with Polar Protic Solvents", *Chem. Eur. J*. **2017**, *23*, 4669-4679. DOI:10.1002/chem.201606012
	100	N. Ando, N.; Fukazawa, A.; Kushida, T.; Shiota, Y.; Itoyama, S.; Yoshizawa, K.; Matsui, Y.; Kuramoto, Y.; Ikeda, H.; Yamaguchi, S. "Photochemical Intramolecular C–H Addition of Dimesityl-(hetero)arylboranes via a [1,6]-Sigmatropic Rearrangement" *Angew. Chem. Int. Ed*., **2017**, *56*, 12210-12214. DOI:10.1002/anie.201706929

様式－ 2

研究業績等

氏名　塩田　淑仁

平成30年3月27日現在

区分	番号	事項
【原著論文】	101	Tsuji, T., Zaoputra, A.A., Hitomi, Y., Mieda, K., Ogura, T., Shiota, Y., Yoshizawa, K., Sato, H., Kodera, M., "Specific Enhancement of Catalytic Activity by a Dicopper Core: Selective Hydroxylation of Benzene to Phenol with Hydrogen Peroxide" *Angew. Chem. Int. Ed.,* **2017**, *56*, 7779-7782. DOI: 10.1002/anie.201702291
	102	Hoshi, K.; Tahara, A.; Sunada, Y.; Tutumi, H.; Inoue, R.; Tanaka, H.; **Shiota, Y.**; Yoshizawa, K.; Nagashima, H., " σ -CAM Mechanisms for the Hydrogenation of Alkenes by cis- and trans-Disilametallacyclic Carbonyl Complexes (M = Fe, Ru, Os): Experimental and Theoretical Studies", *Bull. Chem. Soc. Jpn.* **2017**, *90*, 613-626. DOI:10.1246/bcsj.20170004
	103	Wang, Y., Harada, T., Shiota, Y., Yoshizawa, K., Wang, H., Wang, S., Ye, X., Ogasawara, M., Nakano, T. "Isolation and phototransformation of enantiomerically pure iridium(III) bis[(4,6-difluorophenyl)pyridinato-N,C2]picolinate" *RSC AdV.*, **2017**, *7,* 29550-29553. DOI: 10.1039/c7ra04141a
	104	Tian, H., Shimakoshi, H., Imamura, K., **Shiota, Y.,** Yoshizawa, K., Hisaeda, Y., "Photocatalytic alkene reduction by a B12-TiO2hybrid catalyst coupled with C-F bond cleavage for: Gem -difluoroolefin synthesis" *Chem. Commun.* **2017**, *53*, 9478-9481. DOI: 10.1039/c7cc04377e
	105	Fujita, D., Sugimoto, H., **Shiota, Y**., Morimoto, Y., Yoshizawa, K., Itoh, S., "Catalytic C-H amination driven by intramolecular ligand-to-nitrene one-electron transfer through a rhodium(III) centre" *Chem. Commun.* **2017**, *53*, 4849-4852. DOI: 10.1039/c7cc01840a
	106	Suzuki, W., Kotani, H., Ishizuka, T., Shiota, Y., Yoshizawa, K., Kojima, T. "Formation of supramolecular hetero-triads by controlling the hydrogen bonding of conjugate bases with a diprotonated porphyrin based on electrostatic interaction" *Chem. Commun.* **2017**, *53*, 6359-6362. DOI: 10.1039/c7cc03635c
	107	Yoshizawa, K.; Semoto, T.; Hitaoka, S.; Higuchi, C.; **Shiota, Y.**; Tanaka, H., "Synergy of Electrostatic and van der Waals Interactions in the Adhesion of Epoxy Resin with Carbon-Fiber and Glass Surfaces", *Bull. Chem. Soc. Jpn.*, **2017**, *90*, 500-505. DOI: 10.1246/bcsj.20160426
	108	Saegusa, Y.; Ishizuka, T.; **Shiota, Y.**; Yoshizawa, K.; Kojima, T., "Acid-Base Properties of a Freebase Form of a Quadruply-Ring-Fused Porphyrin—Stepwise Protonation Induced by Rigid Ring-Fused Structure" *J. Org. Chem.*, **2017**, *82*, 322-330. DOI: 10.1021/acs.joc.6b02419
	109	Mahyuddin, M.H., Staykov, A., **Shiota, Y**., Miyanishi, M., Yoshizawa, K. "Roles of Zeolite Confinement and Cu-O-Cu Angle on the Direct Conversion of Methane to Methanol by $[Cu_2(\mu\text{-}O)]^{2+}$-Exchanged AEI, CHA, AFX, and MFI Zeolites" *ACS Catal.* **2017**, *7*, 3741-3751. DOI: 10.1021/acscatal.7b00588
	110	Koide, T., Takesue, M., Murafuji, T., Satomi, K., Suzuki, Y., Kawamata, J., Terai, K., Suzuki, M., Yamada, H., **Shiota, Y**., Yoshizawa, K., Tani, F. "An Azulene-Fused Tetracene Diimide with a Small HOMO–LUMO Gap" *ChemPlusChem,* **2017**, *82*, 1010-1014. DOI: 10.1002/cplu.201600356
	111	Mahyuddin, M.H., **Shiota, Y.**, Staykov, A., Yoshizawa, K. "Theoretical Investigation of Methane Hydroxylation over Isoelectronic $[FeO]^{2+}$- and $[MnO]^{+}$-Exchanged Zeolites Activated by N_2O" *Inorg. Chem.* **2017**, *56*, 10370-10380. DOI:10.1021/acs.inorgchem.7b01284
	112	Kawanami, T., Ishizuka, K., Furuno, H., **Shiota, Y**., Yoshizawa, K., Inanaga, J. "Efficient1H NMR chiral discrimination of sulfoxides caused by the dynamic nature of (R,R)-3',3"-biBINOL" *Tetrahedron Asymm.*, **2017**, *28*, 1587-1590. DOI: 10.1016/j.tetasy.2017.10.008
	113	Hori, Y., **Shiota, Y**., Tsuji, T., Kodera, M., Yoshizawa, K. Catalytic Performance of a Dicopper-Oxo Complex for Methane Hydroxylation *Inorg. Chem.*, **2018**, 57 8-11. DOI: 10.1021/acs.inorgchem.7b02563

（注）用紙が不足する場合は，この様式をコピーしてください

様式- 2

研究業績等

氏名　塩田　淑仁

平成30年3月27日現在

区分	番号	事項
【特許】		
【総説・解説】	1	総説　メタン活性化-電子状態理論からのアプローチ- 触媒55巻3号
【著書】	1	山口兆, 増田秀樹, 榊茂好編、塩田淑仁, 吉澤一成、三共出版、錯体化学選書１０　金属錯体の量子•計算化学、2014、529ページ、（３章　“金属錯体の構造、反応性および生物無機化学反応”195-318ページ）
【招待講演】	1	密度汎関数理論による触媒・酵素反応へのアプローチ、第２回物質合成シンポジウム、2007年1月15日、京都
	2	理論化学は酵素反応をどこまで明らかにできるのか？-数原子のモデルから数万原子の現実系への拡張、第46回日本生物物理学会、2008年12月3日～12月5日、福岡
	3	金属錯体のスピン交差に関する理論的研究、九重分光セミナー2010、2010年7月30日、大分
	4	高原子価金属オキソ種の電子状態とその反応性に関する量子化学計算、第６回稲盛フロンティア研究講演会、2011 年１月５日、福岡
【競争的資金取得状況】	1	**分担** 大規模密度汎関数計算による生体化学反応へのアプローチ、〇吉澤一成、塩田淑仁、科学研究費基盤研究(B)、2002年度-2004年度、10,700千円
	2	**分担** 量子化学計算による生物無機化学の新たな展開、〇吉澤一成、塩田淑仁、科学研究費基盤研究(B)、2006年度-2008年度、14,900千円
	3	**代表** 銅タンパク質による酸素活性化と量子化学計算の新展開、〇塩田淑仁、科学研究費若手研究(B) 2009-2012、4,160千円
	4	**分担**動的キラリティー制御を基盤とする新規キラルシステムの開発：らせんダイナミクスと分子素子機能、〇古野裕史、塩田淑仁、五島健太、九州大学G-COEプログラム科研費、2009年度、1,500千円
	5	**代表** バイオフォトニクスのためのホローファイバの構造設計と機能制御、〇塩田淑仁、徳田陽明、京都大学化学研究所（化学関連分野の深化・連携を基軸とする先端・学際研究拠点)、2010年度、1,200千円
	6	**分担** 量子化学計算による人工変異酵素の設計と反応制御〇吉澤一成、塩田淑仁、蒲池高志、科学研究費基盤研究(A) 2010年度-2014年度、38,090千円
	7	**代表** 酵素触媒反応の原動力となる金属活性種と量子化学計算の新展開、〇塩田淑仁、科学研究費基盤研究(C) 2013 年度-2015 年度、4,100 千円
	8	**代表** 鉄と銅を基軸とした酸素活性化触媒の理論研究、〇塩田淑仁、科学研究費基盤研究(C) 2016 年度-2020 年度、4,550 千円
【研究分野】		理論化学　計算化学　触媒化学
【外部サイト】		ORCID https://orcid.org/0000-0003-2054-9845 Scopus Author ID: 7005590954 https://www.scopus.com/authid/detail.uri?origin=resultslist&authorId=7005590954

（注）用紙が不足する場合は，この様式をコピーしてください