様式－ 2

研究業績等

氏名　塩田　淑仁

平成28年7月20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.
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（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

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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.
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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.
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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.
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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
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	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
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	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

様式－ 2

研究業績等

氏名　塩田　淑仁

平成28年　7月20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*, July 12. DOI: 10.1021/jacs.6b03785
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	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**, *in press*.

（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28年　7月20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、○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、○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、○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、○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、○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○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、○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、○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

（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