

平成22年度 研究業績

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1. 発表論文等 (査読付き論文, 著書, 総説等の発表状況)

- (1) “Marking” the nitrogen atoms of phenyl-(2-pyridyl)-(3-pyridyl)-(4-pyridyl)-methane. Synthesis and absolute configuration of the corresponding tris(pyridine *N*-oxide)  
Matsumoto, K.\*; Miki, K.; Inagaki, T.; Nehira, T.\*; Pescitelli, G.; Hirao, Y.; Kurata, H.; Kawase, T.; Kubo, T.\*, *Chirality*, in press.
- (2) Alternating Covalent Bonding Interactions in a One-Dimensional Chain of a Phenalenyl-Based Singlet Biradical Molecule Having Kekulé Structures  
Shimizu, A.; Kubo, T.\*; Uruichi, M.; Yakushi, K.; Nakano, M.; Shiomi, D.; Sato, K.; Takui, T.; Hirao, Y.; Matsumoto, K.; Kurata, H.; Morita, Y.; Nakasuji, K. *J. Am. Chem. Soc.* **2010**, *132*, 14421–14428.
- (3) Synthesis and Characterization of Teranthene: A Singlet Biradical Polycyclic Aromatic Hydrocarbon Having Kekulé Structures  
Konishi, A.; Hirao, Y.; Nakano, M.; Shimizu, A.; Botek, E.; Champagne, B.\*; Shiomi, D.; Sato, K.; Takui, T.; Matsumoto, K.; Kurata, H.; Kubo, T.\* *J. Am. Chem. Soc.* **2010**, *132*, 11021–11023.
- (4) Singlet Diradical Character from Experiment  
Kamada, K.\*; Ohta, K.; Shimizu, A.; Kubo, T.\*; Kishi, R.; Takahashi, H.; Botek, E.; Champagne, B.; Nakano, M.\* *J. Phys. Chem. Lett.* **2010**, *1*, 937–940.
- (5) Hydrogen-Bonded Quartz-type Network of Diprotonated Tetrakis(4-pyridyl)methane Dications  
Matsumoto, K.\*; Inokuchi, D.; Hirao, Y.; Kurata, H.; Kubo, T.\*, *Cryst. Growth Des.* **2010**, *10*, 2854–2856.
- (6) Pentaleno[1,2-*c*:4,5-*c'*]dithiophene Derivatives: First Synthesis, Properties, and a Molecular Structure  
Konishi, A.; Fujiwara, T.; Ogawa, N.; Hirao, Y.; Matsumoto, K.; Kurata, H.; Kubo, T.; Kitamura, C.; Kawase, T.\* *Chem. Lett.* **2010**, *39*, 300–301.
- (7) Electronic structure of delocalized singlet biradical Ph<sub>2</sub>-IDPL solid film  
Kanai, K.\*; Noda, Y.; Kato, K.; Kubo, T.; Iketaki, K.; Shimizu, A.; Ouchi, Y.; Nakasuji, K.; Seki, K. *Phys. Chem. Chem. Phys.* **2010**, *12*, 12570–12577.

- (8) Dinaphthopentalenes: Pentalene Derivatives for Organic Thin-Film Transistors  
Kawase, T.\*; Fujiwara, T.; Kitamura, C.; Konishi, A.; Hirao, Y.; Matsumoto, K.; Kurata, H.; Kubo, T.; Shinamura, S.; Mori, H.; Miyazaki E.; Takimiya, T.\* *Angew. Chem. Int. Ed.* **2010**, *49*, 7728–7732.
- (9) Giant electric field effect on the second hyperpolarizability of symmetric singlet diradical molecules  
Nakano, M.\*; Champagne, B.; Botek, E.; Ohta, K.; Kamada, K.; Kubo, T. *J. Chem. Phys.* **2010**, *133*, 154302-1–15.
- (10) Signature of multiradical character in second hyperpolarizabilities of rectangular graphene nanoflakes  
Nagai, H.; Nakano, M.\*; Yoneda, K.; Kishi, R.; Takahashi, H.; Shimizu, A.; Kubo, T.; Kamada, K.; Ohta, K.; Botek, E.; Champagne, B. *Chem. Phys. Lett.* **2010**, *489*, 212–218.
- (11) Singlet Open-Shell Character of Polyperiacenes  
Shimizu, A.; Konishi, A.; Hirao Y.; Kubo T. In *Graphene and its Fascinating Attributes*; Swapan, P.; Enoki, T.; Rao, C. N. R. Eds.; World Scientific Publisher: Place of Publication, 2011; Chapter 3, pp 46–57.

## 2. 学会発表等（国内外の招待講演および国際会議での発表状況）

- (1) Synthesis and Investigation of Anti-Ferromagnetic State of Polycyclic Aromatic Hydrocarbons  
Kubo, T.\* Graphene Workshop in Tsukuba, Tsukuba, Japan, 2011.1.17–18（招待講演）.
- (2) Experimental consideration on intermolecular spin-spin interaction of delocalized singlet biradicals  
Kubo, T.\* The 2010 International Chemical Congress of Pacific Basin Societies (Pacifichem 2010), Honolulu, Hawaii, USA, 2010.12.15–20（招待講演）.
- (3) Coupling nature of two electrons in bisanthroxyls  
Kubo, T.\* The 2010 International Chemical Congress of Pacific Basin Societies (Pacifichem 2010), Honolulu, Hawaii, USA, 2010.12.15–20（招待講演）.
- (4) Synthesis and properties of 2,2'-bis(spirodienone)-bridged-3,3'-bithiophene derivatives – An unusual redox behavior caused by ring-opening  
Kurata, H.\*; Fujimoto, T.; Atsuji, Y.; Hirao, Y.; Matsumoto, K.; Kubo, T. The 2010 International Chemical Congress of Pacific Basin Societies (Pacifichem 2010), Honolulu, Hawaii, USA, 2010.12.15–20（ポスター発表）.

- (5) Stabilization and isolation of anthroxyl radical species  
Hirao, Y.\*; Saito, T.; Konishi, A.; Matsumoto, K.; Kurata, H.; Kubo, T. The 2010 International Chemical Congress of Pacific Basin Societies (Pacifichem 2010), Honolulu, Hawaii, USA, 2010.12.15–20 (ポスター発表).
- (6) Synthesis and properties of teranthene: Onset of “edge state” in molecular-sized nanographene molecule  
Konishi, A.\*; Shimizu, A.; Hirao, Y.; Matsumoto, K.; Kurata, H.; Kubo, T. The 2010 International Chemical Congress of Pacific Basin Societies (Pacifichem 2010), Honolulu, Hawaii, USA, 2010.12.15–20 (ポスター発表).
- (7) Studies of a phenalenyl-based molecule with triradical character  
Aoba, M.\*; Shimizu, A.; Hirao, Y.; Matsumoto, K.; Kurata, H.; Kubo, T. The 2010 International Chemical Congress of Pacific Basin Societies (Pacifichem 2010), Honolulu, Hawaii, USA, 2010.12.15–20 (ポスター発表).
- (8) Synthetic studies of cage-shaped oligothiophene  
Kurata, H.; Adachi, K.\*; Hirao, Y.; Matsumoto, K.; Kubo, T. The 2010 International Chemical Congress of Pacific Basin Societies (Pacifichem 2010), Honolulu, Hawaii, USA, 2010.12.15–20 (ポスター発表).
- (9) Mechanochromism of 2,2'-Bis(spirodienone)-Bridged-3,3'-Bithiophene Derivatives  
Kurata, H.; Atsuji, Y.\*; Hirao, Y.; Matsumoto, K.; Amimoto, K.; Kubo, T. The 2010 International Chemical Congress of Pacific Basin Societies (Pacifichem 2010), Honolulu, Hawaii, USA, 2010.12.15–20 (ポスター発表).
- (10) Studies on the synthesis and properties of dendrimer molecule based on tetrakis(2-thienyl)methane framework  
Kugo, S.\*; Matsumoto, K.; Takajo, D.; Hirao, Y.; Kurata, H.; Kubo, T. The 2010 International Chemical Congress of Pacific Basin Societies (Pacifichem 2010), Honolulu, Hawaii, USA, 2010.12.15–20 (ポスター発表).
- (11) Crystal structure and solid state properties of quartz type hydrogen bonded network of tetrakis(4-pyridyl)methane dication  
Inokuchi, D.\*; Matsumoto, K.; Hirao, Y.; Kurata, H.; Kubo, T. The 2010 International Chemical Congress of Pacific Basin Societies (Pacifichem 2010), Honolulu, Hawaii, USA, 2010.12.15–20 (ポスター発表).

- (12) Synthesis of the novel ligands based on tetrakis(2-pyridyl)- methane and their metal complexes  
Kawashita, K.\*; Matsumoto, K.; Hirao, Y.; Kurata, H.; Kubo T. The 2010 International Chemical Congress of Pacific Basin Societies (Pacifichem 2010), Honolulu, Hawaii, USA, 2010.12.15–20 (ポスター発表).
- (13) 開殻電子構造を有する縮合多環芳香族化合物の合成と性質  
久保 孝史\*, 第4回有機 $\pi$ 電子系シンポジウム, シーパル須磨, 兵庫, 2010.11.9–10 (招待講演).
- (14) Anti-ferromagnetic State of Conjugated Kekulé Molecules  
Kubo, T.\*; Shimizu, A.; Hirao, T.; Matsumoto, K.; Kurata, H.; Nakano, M. International Conference on Science and Technology of Synthetic Metals (ICSM2010), Kyoto, Japan, 2010.7.4–9
- (15) Electronic Structures and Solid State Properties of Oligoynes-Bridged Bisphenalenyl  
Hirao, Y.\*; Ishida, M.; Daifuku, Y.; Matsumoto, K.; Kurata, H.; Kubo, T. International Conference on Science and Technology of Synthetic Metals (ICSM2010), Kyoto, Japan, 2010. 7. 4–9
- (16) Crystal Structure and Properties of the Salts of Diprotonated Tetrakis(4-pyridyl)methane  
Inokuchi, D.; Matsusmoto, K.; Hirao, Y.; Kurata, H.; Kubo, T. International Conference on Science and Technology of Synthetic Metals (ICSM2010), Kyoto, Japan, 2010. 7. 4–9

### 3. 特許

特になし

### 4. 学会・シンポジウム等の開催状況

- (1) The 2010 International Chemical Congress of Pacific Basin Societies (Pacifichem 2010):  
Designed pi-Electronic Systems: Synthesis, Properties, Theory and Function (#29),  
Honolulu, Hawaii, USA, 2010.12.15–20, Michael Haley(chief organizer), Takashi Kubo  
(co-organizer), Graham Bodwell (co-organizer), Yoshito Tobe (co-organizer)

## 5. 受賞等

(1) 猪口大輔 (博士 2 年)

Young Researcher Poster Award, International Conference on Science and Technology of Synthetic Metals 2010 (ICSM 2010), 2010. 7.6

(2) 小西彬仁 (博士 1 年)

ポスター賞 第 42 回構造有機若手の会, 2010.8.8

(3) 青葉充哉 (修士 2 年)

ポスター賞 第 42 回構造有機若手の会, 2010.8.8

(4) 齋藤 徹 (修士 1 年)

ポスター賞 第 42 回構造有機若手の会, 2010.8.8

(5) 石田恵 (修士 1 年)

ポスター賞 第 4 回有機πシンポジウム, 2010.11.19

## 6. 新聞報道等

(1) **Highlighted by Prof. Christoph Lambert in ANGEW. CHEM. INT. ED.** (*Angew. Chem. Int. Ed.* **2011**, 50, 1756–1758)

Synthesis and Characterization of Teranthene: A Singlet Biradical Polycyclic Aromatic Hydrocarbon Having Kekulé Structures

Konishi, A.; Hirao, Y.; Nakano, M.; Shimizu, A.; Botek, E.; Champagne, B.\*; Shiomi, D.; Sato, K.; Takui, T.; Matsumoto, K.; Kurata, H.; Kubo, T.\* *J. Am. Chem. Soc.* **2010**, 132, 11021–11023.

(2) **Selected by the Editorial Board of SYNFACTS** (*Synfacts* **2010**, 11, 1238)

Synthesis and Characterization of Teranthene: A Singlet Biradical Polycyclic Aromatic Hydrocarbon Having Kekulé Structures

Konishi, A.; Hirao, Y.; Nakano, M.; Shimizu, A.; Botek, E.; Champagne, B.\*; Shiomi, D.; Sato, K.; Takui, T.; Matsumoto, K.; Kurata, H.; Kubo, T.\* *J. Am. Chem. Soc.* **2010**, 132, 11021–11023.

(3) **Selected by the Editorial Board of SYNFACTS** (*Synfacts* **2010**, 5, 0530)

Synthesis and Identification of a Trimethylenemethane Derivative p-Extended with Three pyridinyl Radicals

Matsumoto, K.; Inokuchi, D.; Hirao, Y.; Kurata, H.; Sato, K.; Takui, T.; Kubo, T. *Org. Lett.* **2010**, 12, 836–839.

## 7. 領域内の共同研究の準備・実施状況とその成果

(1) 共同研究先：物質・材料研究機構ナノ有機センター，三木一司グループ（A01 班，公募班員）

派遣人員（受入）：

派遣期間（受入）：

共同研究内容：フロー系二光子吸収を用いた芳香族縮環反応の開発

共同研究成果：サンプルを提供し，反応条件を現在検討中

## 8. その他特記事項

特になし