

# SCIENCE BULLETIN OF JOSAI UNIVERSITY

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城西大学理学部研究報告

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FACULTY OF SCIENCE  
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# **SCIENCE BULLETIN OF JOSAI UNIVERSITY**

**城西大学理学部研究報告**

**Vol. 24 March 2018**

## **Editorial Board**

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*PART I ANNUAL REPORTS*

# 1. Abstracts of Papers Published in Journals

## MATHEMATICS

### Drawing Curves

T. Oshima

*Mathematical Progress in Expressive Image Synthesis III*, edited by Y. Dobashi and H. Ochiai, *Mathematics for Industry* **24** (2016), 95-106, Springer.

A method drawing curves is proposed. A program drawing graphs of mathematical functions using this method is realized in a computer algebra and outputs the graphs in a source file of T<sub>E</sub>X and then transforms it into a PDF file.

### On convergence of basic hypergeometric series

T. Oshima

*Josai Mathematical Monographs* **10** (2017), 215-223.

We examine the convergence of  $q$ -hypergeometric series when  $|q| = 1$ . We give a condition so that the radius of the convergence is positive and get the radius. We also show that the numbers  $q$  with the positive radius of the convergence are densely distributed in the unit circle  $|q| = 1$  and so are those with the radius 0.

### Reducibility of hypergeometric equations

T. Oshima

*Analytic, Algebraic and Geometric Aspects of Differential Equations, Trends in Mathematics*, 425-435, 2017, Birkhäuser.

We study a necessary and sufficient condition so that hypergeometric equations are reducible. Here the hypergeometric equations with one variable mean the rigid Fuchsian linear ordinary differential equations. If the equations with one variable have more than four singular points, they naturally define hypergeometric equations with several variables including Appell's hypergeometric equations. We also study the reducibility of such equations with several variables and we find a new kind of reducibility, which appears, for example, in a decomposition of Appell's  $F_4$ .

### Transformation of KZ type equations

T. Oshima

*Microlocal Analysis and Singular Perturbation Theory, RIMS Kôkyûroku Bessatsu B61 (2017), 141-162.*

The middle convolution introduced by Katz is extended to an operation on a regular holonomic system by Haraoka. We study this operation on a KZ type equation and we clarify how the conjugacy classes of resulting residue matrices under this operation are determined in terms of the original residue matrices and examine the relation with other related transformations.

### 立体モデルおよびスライド・タブレットを併用した数学教材の開発

濱口直樹<sup>\*1</sup>, 大島利雄, 高遠節夫<sup>\*2</sup> (\*1 長野高専一般科, \*2 東邦大学理学部)  
城西大学数学科 教職課程紀要, 1(2) (2017), 2006-2013.

### Some properties of spaces associated with sub-Hankel determinants, Analysis, Geometry and Representations on Lie Groups and Homogeneous Spaces.

Hideyuki Ishi<sup>\*1</sup>, Takeyoshi Kogiso (\*1 Department of Mathematics, Nagoya University)  
*Analysis, Geometry and Representations on Lie Groups and Homogeneous Spaces, Seminar on Mathematical Sciences, Keio Univ. 2016., No. 39, pp. 83-94. (SSN: 1880-6511)*

In this note, we show that the space associated with sub-Hankel determinant is a non-reductive, regular prehomogeneous vector space, and we give the multiplicative Legendre transforms of sub-Hankel determinants. Moreover we observe certain relations between b-functions of polarization of PV-polynomials and b-functions of sub-Hankel determinants, and give some formulas about sub-Hankel determinants whose components are orthogonal polynomials.

### Clifford quartic forms and local functional equations of non-prehomogeneous type.

Takeyoshi Kogiso, Fumihiko Sato<sup>\*1</sup>, (\*1 Department of Mathematics, Rikkyo University)  
*J. Math. Sci Univ. Tokyo, 23 (2016), 791-866.*

It is known that one can associate local zeta functions satisfying a functional equation to the irreducible relative invariant of an irreducible regular prehomogeneous vector space. We construct polynomials of degree 4 (called *Clifford quartic forms*) that cannot be obtained from prehomogeneous vector spaces, but for which one can associate local zeta functions satisfying functional equations. The Clifford quartic form is defined for each finite dimensional representation of the tensor product of the Clifford algebras of two positive definite real quadratic

forms and cannot be a relative invariant of any prehomogeneous vector space except for a few low dimensional cases. We also classify the exceptional cases of small dimension, namely, we determine all the prehomogeneous vector spaces with Clifford quartic forms as a relative invariant.

### **Pairs of polynomials which satisfy the local functional equations.**

Takeyoshi Kogiso

*Josai Mathematical Monograph*, vol. 10. (2016).

In this note, we survey the fundamental theorem of prehomogeneous vector spaces which is related to the local functional equations of polynomials and announce a recent result of this field.

### **Compact homogeneous locally conformally Kähler manifolds**

Y. Kamishima, K. Hasegawa

*Osaka J. Math.* **53** (2016), 683-703.

We have proved that every compact homogeneous locally conformally Kähler (*lcK* for short) manifold  $M$  has a structure of holomorphic principal fiber bundle over a flag manifold with fiber a 1-dimensional complex torus.  $M$  must be a Vaisman manifold. A Lie group appearing in homogeneous manifold  $M$  is a compact reductive Lie group. Then we determine *lcK* reductive Lie groups and compact locally homogeneous *lcK* manifolds of reductive Lie groups.

### **On quaternionic 3 CR-structure and pseudo-Riemannian metric**

Y. Kamishima

*Applied Math.* **9**(2) (2018) 114-129 (*Special Issue on Riemannian Geometry*), (2018).

A *CR*-structure on a  $2n+1$ -manifold gives a conformal class of Lorentz metrics on the Fefferman  $S^1$ -bundle. This analogy is carried out to the *quaternionic conformal 3-CR structure* (a generalization of quaternionic *CR*-structure) on a  $4n+3$ -manifold  $M$ . This structure produces a conformal class  $[g]$  of a pseudo-Riemannian metric  $g$  of type  $(4n+3, 3)$  on  $M \times S^3$ . Let  $(\mathrm{PSp}(n+1, 1), S^{4n+3})$  be the geometric model obtained from the projective boundary of the complete simply connected quaternionic hyperbolic manifold. We shall prove that  $M$  is locally modeled on  $(\mathrm{PSp}(n+1, 1), S^{4n+3})$  if and only if  $(M \times S^3, [g])$  is conformally flat (i.e. the Weyl conformal curvature tensor vanishes).



## Two aspects of the theta divisor associated with the autonomous Garnier system of type 9/2

A. Nakamura

*JMM 10* (2017), Representation Theory and Differential Equations, 193-214.

We consider the autonomous Garnier system of type 9/2 as an example to illustrate the possible correspondence from the nonlinear to the linear equation by studying generic degeneration of the theta divisor of the Liouville tori and the spectral curve.

### アクティブラーニングによる図形と理論に関する学習の例

小木曾岳義, 清水優祐, 中村あかね, 廣恵一希

平成 29 年城西大学数学科教職課程紀要, 城西大学数学教室, 第 1 巻 1 号 (2017) 1107-1115

学習内容をより効果的に印象に残るように指導した, 図形と論理に関する教材を用いたアクティブラーニングの例と, その教育効果について紹介した。

## PHYSICS

### Transfer Excitation Processes Observed in $N^{3+}$ -He and $O^{3+}$ -He Collisions at $E_{lab} = 33$ eV

Yoh Itoh

*J. Phys. Soc. Jpn.* **85**, 094301 (7 pages) (2016)

[http://libir.josai.ac.jp/il/meta\\_pub/G0000284repository\\_JOS-JPSJ.85.094301](http://libir.josai.ac.jp/il/meta_pub/G0000284repository_JOS-JPSJ.85.094301)

State-selective differential cross sections (DCSs) for the following reactions were reported:  $N^{3+} (1s^2 2s^2 1S) + He (1s^2 1S) \rightarrow N^{2+} (1s^2 2s2p^2 2D) + He^+ (1s^2 S) + 10.3$  eV,  $O^{3+} (1s^2 2s^2 2p^2 P) + He (1s^2 1S) \rightarrow O^{2+} (1s^2 2s 2p^3 3P) + He^+ (1s^2 S) + 12.7$  eV, and  $O^{3+} (1s^2 2s^2 2p^2 P) + He (1s^2 1S) \rightarrow O^{2+} (1s^2 2s 2p^3 3D) + He^+ (1s^2 S) + 15.5$  eV. The scattering angle  $\theta_{lab}$  studied in the laboratory frame ranged from  $-3.0$  to  $22^\circ$  and the laboratory collision energy  $E_{lab}$  was 33 eV. Only the transfer excitation processes, i.e., the electron capture reactions with the simultaneous excitation of the projectile, were found to be the main channels for one-electron capture reactions in these systems. A classical trajectory analysis within the two-state approximation based on the ab initio potentials for  $(NHe)^{3+}$  revealed that the transfer excitation of a two-electron process takes place through a single crossing of the relevant potentials.

## CHEMISTRY

### TD DFT 法による OHBA の吸光・発光スペクトルの理論的研究

新井健文, 長岡伸一<sup>\*1</sup>, 長嶋雲兵<sup>\*2</sup>, 寺前裕之 (\*1 愛媛大, \*2 産総研)

*J. Comp. Chem. Jpn.* **14**, 209-210 (2015) (日本コンピューター化学会秋季年会 2015 年精選論文特

集選出)

We have studied the first excited state of *o*-hydroxybenzaldehyde with TD DFT calculations. We have attempted systematic calculations to select a proper functional to describe the correlation between the absorption and emission spectra and the Hammett's  $\sigma$  values. The results with XAB95 functional are considered to be near the experimental results of the emission spectra.

## 2-アザスピロ環化合物における閉環反応の理論的研究

寺前裕之, 須田 岬, 湯川 満, 林 浩輔<sup>\*1</sup>, 高山 淳<sup>\*1</sup>, 坂本武史<sup>\*1</sup> (\*1 城西大薬)  
*J. Comp. Chem. Jpn.*, **14**, 213-214 (2015) (日本コンピューター化学会秋季年会 2015 年精選論文特集選出)

The geometric structures of the phenoxenium cation which is a cation intermediate of 2-azaspiro ring compounds (2-azaspiro[4.5]decane) from *N*-methoxy-*N*-prenylbenzamide are studied by means of the Hamiltonian algorithm with ab initio molecular orbital calculations at HF/3-21G level. The geometries are further refined with MP2/6-311G<sup>\*\*</sup> level. We tried four substituted compounds with the methyl group. Among them only one compound with two methyl groups gives a ring-closure intermediate, which agrees well with the experimental results.

## Theoretical study on the structures of ethanolamine and its water complexes using the Hamiltonian algorithm

Hiroyuki Teramae, Yasuko Y. Maruo<sup>\*1</sup> (\*1 Tohoku Institute of Technology)  
*AIP Conference Proceedings* **1702**, 090041 (2016); doi:<http://doi.org/10.1063/1.4938849>

We try to optimize the structures of monoethanolamine (MEA), MEA dimer, MEA + two water molecules, and MEA dimer + four water molecules as the model of MEA in aqueous solutions using the Hamiltonian algorithm. We found the most stable MEA backbones are all gauche structures. The MEA in aqueous solution seems to exist as dimer or larger aggregates. As the base, the water molecule would be more important than another MEA because of the hydrogen bond networks.

## Practical Training on Adding Polarization and Diffuse Functions to Basis Set for Molecular Orbital Calculation

S. Nagaoka<sup>\*1</sup>, H. Teramae, U. Nagashima<sup>\*2</sup> (\*1 Ehime University, \*2 FOCUS)  
*Aust. J. Educ. Chem.* **75**, 8-15 (2016)

Adding a polarization function to a basis set for a molecular orbital calculation is fre-

quently useful for producing accurate representations of chemical bonding. Adding a diffuse function is also important when considering anions. This article explains practical training that could greatly promote intuitive understanding of the general idea of adding these functions. In the training, students draw contour plots of molecular orbitals supplemented with and without each of the polarization and diffuse functions by using Microsoft Excel and visualize the effect of each addition.

### **Hamiltonian algorithm and its application to the aromatic oxidative cyclization on *N*-methoxy-*N*-prenylbenzamide**

Hiroyuki Teramae, Kousuke Hayashi<sup>\*1</sup>, Jun Takayama<sup>\*1</sup>, Takeshi Sakamoto<sup>\*1</sup> (\*1 Faculty of Pharmaceutical Sciences, Josai University)

*AIP Conference Proceedings* **1790**, 020024 (2016); <http://doi.org/10.1063/1.4968650>

The geometric structures of the phenoxenium cation which is a cation intermediate of 2-azaspiro ring compounds (2-azaspiro[4.5]decane) from *N*-methoxy-*N*-prenylbenzamide are studied by means of the Hamiltonian algorithm with *ab initio* molecular orbital calculations at HF/3-21G level. The geometries are further refined with MP2/6-311G<sup>\*\*</sup> level. We tried four substituted compounds with the methyl group. Among them only one compound with two methyl groups gives a ring-closure intermediate, which agrees well with the experimental results.

### **Oxidative Dearomatic Cyclization of *N*-Substituted Benzanilide Derivatives: Conformational Effect of Amide Groups on the Reaction**

Kousuke Hayashi<sup>\*1</sup>, Jun Takayama<sup>\*1</sup>, Meiyun Xuan<sup>\*1</sup>, Misaki Suda, Hiroyuki Teramae, Takeshi Sakamoto<sup>\*1</sup> (\*1 Faculty of Pharmaceutical Sciences, Josai University)

*Heterocycles*, **92** (10), 1785–1786 (2016)

The synthesis of spirooxindoles with a hypervalent iodine reagent depended on *N*-substituted benzanilide derivatives as starting materials. Reaction yields of benzanilides containing various *N*-substituents were discovered to relate to the *cis* and *trans* conformations of the amide bond by *ab initio* molecular orbital calculations at the B3LYP/6-31G(d,p) and MP2/6-31G(d,p) levels, including full geometry optimizations. The relationship between the reaction and conformation of the starting material by quantum chemical calculations was applied to the formal synthesis of SR121463.

### **結晶軌道法による DNA の Hartree-Fock 計算の試み**

寺前裕之, 青木百合子<sup>\*1</sup> (\*1 九大)

*J. Comp. Chem. Jpn*, **15**, 219–220 (2016) (日本コンピューター化学会秋季年会 2016 年精選論文特集選出)

As an attempt at the electronic structure calculations of the B-type model-DNA, (poly-(guanine) poly-(cytosine)) model polymers is performed by means of ab initio crystal orbital method adapting the screw axis-symmetry which results in great reduction of computational efforts. All sugar backbones and ions are included in the calculations. Energy band structures are calculated at 3-21G and 6-31G levels. The effective mass of hole shows a relatively large value while that of electron shows a smaller value which suggests electron conduction in the DNA backbones.

### **An Attempt at Ab Initio Crystal Orbital Calculation of Electronic Structure of B-type Model-DNA**

Hiroyuki Teramae, Yuriko Aoki<sup>\*1</sup> (\*1 Kyushu University)

*AIP Conference Proceedings* **1906**, 030023 (2017); <https://doi.org/10.1063/1.5012302>

As an attempts at the electronic structure calculations of the B-type model-DNA, (poly-(guanine) poly-(cytosine)) double helix including sodium atoms as counter cation, hereafter referred as (poly-(dG)poly-(dC), double helix model polymer is performed by means of *ab initio* Hartree-Fock crystal orbital method adapting the screw axis symmetry which results in great reduction of computational efforts. All sugar backbones and ions are included in the calculations. Energy band structures are calculated at 3-21G and 6-31G levels. It is significant that the bottom of the lowest conduction band at the  $\Gamma$  point of the first Brillouin zone has almost zero energy value. The effective masses of the hole and electron at the  $\Gamma$  point is 13.7 and 9.53. Both values are relatively large, therefore, the band conduction are expected not to be effective in this model-DNA backbone.

### **Practical Training on Adding Polarization Function to Basis Set for Molecular Orbital Calculation of Ethylene**

S. Nagaoka<sup>\*1</sup>, H. Teramae, U. Nagashima<sup>\*2</sup> (\*1 Ehime University, \*2 FOCUS)

*J. Comp. Chem. Jpn. Int. Ed.*, **3**, 2016-0068 (2017)

Adding a polarization function to a basis set for molecular orbital calculation is frequently useful for producing accurate representations of chemical bonding. This article explains practical training that could greatly promote intuitive understanding of the general idea of adding a 3d-type polarization function in a  $\pi$ -type molecular-orbital function. In the training, by using Microsoft Excel, students draw contour plots of the molecular orbitals supplemented with and without the polarization function in ethylene ( $\text{CH}_2 = \text{CH}_2$ ), and visualize the effect of the addition.

**Absorption intensity changes and frequency shifts of fundamental and first overtone bands for OH stretching vibration of methanol upon methanol–pyridine complex formation in carbon tetrachloride: analysis by near-infrared/infrared spectroscopy and density functional theory calculations**

Y. Futami<sup>\*1</sup>, Y. Ozaki and Y. Ozaki<sup>\*2</sup> (\*1 Kumamoto National College of Technology, \*2 Kwansai Gakuin University)

*Phys. Chem. Chem. Phys.*, **18**, 5580–5586 (2016).

Infrared (IR) and near infrared (NIR) spectra were measured for methanol and methanol–pyridine complex in carbon tetrachloride. Upon the formation of the methanol–pyridine complex, the frequencies of both the fundamental and first overtone bands of the OH stretching vibration shifted to lower wavenumbers, and the absorption intensity of the fundamental increased significantly, while that of the first overtone decreased markedly. By using quantum chemical calculations, we estimated the absorption intensities and frequencies of the fundamental and first overtone bands for the OH stretching vibration based on the one-dimensional Schrödinger equation. The calculated results well reproduced the experimental results. The molecular vibration potentials and dipole moment functions of the OH stretching vibration modes were compared between methanol and methanol–pyridine complex in terms of absorption intensity changes and frequency shifts. The large change in the dipole moment function was found to be the main cause for the variations in absorption intensity for the fundamental and first overtone bands.

**Density functional theory study of adsorption geometries and electronic structures of azo-dye-based molecules on anatase TiO<sub>2</sub> surface for dye-sensitized solar cell applications**

Pongthep Prajongtat<sup>\*</sup>, Songwut Suramitr<sup>\*</sup>, Somkiat Nokbin<sup>\*</sup>, Koichi Nakajima<sup>\*\*</sup>, Koichiro Mitsuke, Supa Hannongbua<sup>\*</sup> (\*Kasetsart University, \*\*Hosei University)

*J. Mol. Graph. Model.* **76**, 551–561 (2017)

Structural and electronic properties of eight isolated azo dyes (Ar–N=N–Ar', where Ar and Ar' denote the aryl groups containing benzene and naphthalene skeletons, respectively) were investigated by density functional theory (DFT) based on the B3LYP/6-31G(d,p) and TD-B3LYP/6-311G(d,p) methods. The effect of methanol solvent on the structural and electronic properties of the azo dyes was elucidated by employing a polarizable continuum model (PCM). Then, the azo dyes adsorbed onto the anatase TiO<sub>2</sub> (101) slab surface through a carboxyl group. The geometries and electronic structures of the adsorption complexes were determined using periodic DFT based on the PWC/DNP method. The calculated adsorption energies indicate that the adsorbed dyes preferentially take configuration of the bidentate bridging rather than chelating or monodentate ester-type geometries. Furthermore, the azo compounds having two carboxyl groups are coordinated to the TiO<sub>2</sub> surface more preferentially through the carboxyl group connecting to the benzene skeleton than through

that connecting to the naphthalene skeleton. The dihedral angles ( $\Phi_{B-N}$ ) between the benzene- and naphthalene-skeleton moieties are smaller than  $10^\circ$  for the adsorbed azo compounds containing one carboxyl group. In contrast,  $\Phi_{B-N} > 30^\circ$  are obtained for the adsorbed azo compounds containing two carboxyl groups. The almost planar conformations of the former appear to strengthen both  $\pi$ -electrons conjugation and electronic coupling between low-lying unoccupied molecular orbitals of the azo dyes and the conduction band of  $TiO_2$ . On the other hand, such coupling is very weak for the latter, leading to a shift of the Fermi level of  $TiO_2$  in the lower-energy direction. The obtained results are useful to design and synthesize novel azo-dye-based molecules that give rise to higher photovoltaic performances of the dye-sensitized solar cells.

### **Heterologous expression of thermolabile proteins enhances thermotolerance in *Escherichia coli*.**

Ueda Y., Yamauchi S., Fukata S., Okuyama H., Morita E. H., Shelake R. M. Hayashi, H. *Adv in Microbiol.* **6**(9) 600-612 (2016).

Heat shock proteins (HSPs) play important roles in the mechanism of cellular protection against various environmental stresses. It is well known that accumulation of misfolded proteins in a cell triggers the HSPs expression in prokaryotes as well as eukaryotes. In this study, we heterologously expressed two proteins in *E. coli*, namely, citrate synthase (*CpCSY*) and malate dehydrogenase (*CpMDH*) from a psychrophilic bacterium *Colwellia psychrerythraea* 34H (optimal growth temperature  $8^\circ C$ ). Our analyses using circular dichromism along with temperature-dependant enzyme activities measured in purified or direct cell extracts confirmed that the *CpCSY* and *CpMDH* are thermolabile and present in misfolded form even at physiological growth temperature. We observed that the cellular levels of HSPs, both GroEL and DnaK cheperonins were increased. Similarly, higher levels were observed for sigma factor  $\sigma^{32}$  which is specific to heat-shock protein expression. These results suggest that the misfolded-thermolabile proteins expressed in *E. coli* induced the heat shock response. Furthermore, heat treatment ( $53^\circ C$ ) to wild type *E. coli* noticeably delayed their growth recovery but cells expressing *CpCSY* and *CpMDH* recovered their growth much faster than that of wild type *E. coli*. This reveals that the HSPs expressed in response to misfolded-thermolabile proteins protected *E. coli* against heat-induced damage. This novel approach may be a useful tool for investigating stress-tolerance mechanisms of *E. coli*.

### **Structural analysis and homology modeling of members of *smt*-like operon from thermophilic cyanobacterium *Thermosynechococcus elongatus* BP-1.**

Shelake R.M., Hayashi H., Morita E.H. *Journal of Proteins and Proteomics.* **7**(3), 221-230 (2016).

Whole genome sequencing of several cyanobacteria is recently completed and it offers

a platform to explore metal homeostasis systems in further detail. In the present study, we mined genome of the hot spring cyanobacterium *Thermosynechococcus elongatus* BP-1 for metal sensors and metal-handling proteins. Detailed analysis of the genome data revealed a putative metal (zinc) homeostasis system (*tmt*) in *T. elongatus* BP-1 similar to that of *smt* operon in freshwater *Synechococcus* sp. PCC 7942. The *tmt* operon consists of two genes encoding a transcription regulator (TmtB) and metallothionein (TmtA). Also, transposase gene is exceptionally present in between TmtB and TmtA which is not observed in other *smt*-like operons. Amino acid sequence alignment confirmed that the TmtB shares higher similarity with SmtB (55%) from *Synechococcus* sp. PCC 7942 than another well-studied transcription regulator ZiaR (49%) from *Synechocystis* sp. PCC 6803. Also, important features of ArsR/SmtB family, such as metal-binding ligands and DNA-binding domain in TmtB are highly conserved. Alignment analysis of TmtA showed that the Cys-His residues involved in metal binding are highly conserved. Also, operator/promoter region of *tmtA* consists of an imperfect 12-2-12 inverted repeat which acts as a binding site for ArsR/SmtB transcription regulators. Furthermore, these findings are consistent with our experimental modeling data sets for the predicted secondary and tertiary structures for both the proteins.

### **A novel mechanism of “metal gel-shift” by histidine-rich Ni<sup>2+</sup>-binding Hpn protein from *Helicobacter pylori* strain SS1**

Shelake, R. M., Ito Y., Matsumoto J., Morita, E. H., Hayashi H.  
*PLoS ONE* **12**(2): e0172182, February (2017)

SDS-PAGE is a universally used method for determining approximate molecular weight (MW) in protein research. Migration of protein that does not correlate with formula MW, termed “gel shifting” appears to be common for histidine-rich proteins but not yet studied in detail. We investigated “gel shifting” in Ni<sup>2+</sup>-binding histidine-rich Hpn protein cloned from *Helicobacter pylori* strain SS1. Our data demonstrate two important factors determining “gel shifting” of Hpn, polyacrylamide-gel concentration and metal binding. Higher polyacrylamide-gel concentrations resulted in faster Hpn migration. Irrespective of polyacrylamide-gel concentration, preserved Hpn-Ni<sup>2+</sup> complex migrated faster (3-4 kDa) than apo-Hpn, phenomenon termed “metal gel-shift” demonstrating an intimate link between Ni<sup>2+</sup> binding and “gel shifting”. To examine this discrepancy, eluted samples from corresponding spots on SDS-gel were analyzed by MALDI-TOF-MS. The MW of all samples was the same (6945.66 ± 0.34 Da) and identical to formula MW with or without added mass of Ni<sup>2+</sup>. MALDI-TOF-MS of Ni<sup>2+</sup>-treated Hpn revealed that monomer bound up to six Ni<sup>2+</sup> ions non-cooperatively, and equilibrium between protein-metal species was reliant on Ni<sup>2+</sup> availability. This corroborates with gradually increased heterogeneity of apo-Hpn band followed by compact “metal-gel shift” band on SDS-PAGE. In view of presented data metal-binding and “metal-gel shift” models are discussed.

### Effective derivatization and extraction of insoluble missing lanthanum metallofullerenes La@C<sub>2n</sub> (n = 36-38) with iodobenzene

Yutaka Maeda<sup>\*1</sup>, Takayoshi Tsuchiya<sup>\*2</sup>, Takashi Kikuchi<sup>\*2</sup>, Hidefumi Nikawa<sup>\*2</sup>, Tao Yang<sup>\*3</sup>, Xiang Zhao<sup>\*3</sup>, Zdenek Slanina<sup>\*1</sup>, Mitsuaki Suzuki<sup>\*1,8</sup>, Michio Yamada<sup>\*1</sup>, Yongfu Lian<sup>\*4</sup>, Shigeru Nagase<sup>\*5</sup>, Xing Lu<sup>\*6</sup>, Takeshi Akasaka<sup>\*1,2,6,7</sup> (\*1 Department of Chemistry, Tokyo Gakugei University, \*2 Life Center of Tsukuba Advanced Research Alliance, University of Tsukuba, \*3 Institute for Chemical Physics & Department of Chemistry, State Key Laboratory of Electrical Insulation and Power Equipment, Xi'an Jiaotong University, \*4 Key Laboratory of Functional Inorganic Material Chemistry, Ministry of Education, School of Chemistry and Materials Science, Heilongjiang University, \*5 Fukui Institute for Fundamental Chemistry, Kyoto University, \*6 College of Materials Science and Engineering, Huazhong University of Science and Technology, \*7 Foundation for Advancement of International Science, \*8 Present Addresses: Department of Chemistry, Faculty of Science, Josai University) *Carbon*. **98**. (2016), 67-73.

Insoluble metallofullerenes, La@C<sub>2n</sub> (n = 36-38), was extracted by dichlorobenzene, chlorobenzene, and iodobenzene as a solvent under reflux condition. When iodobenzene was used, La@C<sub>2n</sub> (n = 36-38) was successfully extracted as the corresponding phenyl adducts, such as La@C<sub>72</sub>(C<sub>6</sub>H<sub>5</sub>), La@C<sub>74</sub>(C<sub>6</sub>H<sub>5</sub>), and La@C<sub>76</sub>(C<sub>6</sub>H<sub>5</sub>). The number of isomers of corresponding adducts, La@C<sub>72</sub>(C<sub>6</sub>H<sub>5</sub>) and La@C<sub>74</sub>(C<sub>6</sub>H<sub>5</sub>), were reduced to one-third of that in 1,2,4-trichlorobenzene extracts, which was reported previously. Based on the spectroscopic analysis, the carbon cages of La@C<sub>72</sub>(C<sub>6</sub>H<sub>5</sub>) and La@C<sub>74</sub>(C<sub>6</sub>H<sub>5</sub>) were identified to be La@C<sub>2</sub>(10612)-C<sub>72</sub>(C<sub>6</sub>H<sub>5</sub>) and La@D<sub>3h</sub>-C<sub>74</sub>(C<sub>6</sub>H<sub>5</sub>), respectively.

### Molecular Location Sensing Approach by Anisotropic Magnetism of an Endohedral Metallofullerene

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Location recognition at the molecular scale provides valuable information about the nature of functional molecular materials. This study presents a novel location sensing approach based on an endohedral metallofullerene, Ce@C<sub>82</sub>, using its anisotropic magnetic



properties, which lead to temperature-dependent paramagnetic shifts in  $^1\text{H}$  NMR spectra. Five  $\text{Ce}@C_{82}$  site-isomers derived from mesitylene were synthesized to demonstrate the spatial sensing ability of  $\text{Ce}@C_{82}$ . Single-crystal structures, absorption spectra, and density functional theory calculations were used to select the plausible addition positions in the radical coupling reaction, which preferentially happens on the carbon atoms with high electron density of the singly occupied molecular orbital (SOMO) and positive charge. Unique paramagnetic shifts of the  $^1\text{H}$  peaks, which were derived from the anisotropic magnetism of the f-electron in the Ce atom of the isomers, were observed by temperature-dependent NMR measurements. It was found that the magnetic anisotropy axes can be easily predicted by theoretical calculations using the Gaussian 09 package. Further analysis revealed that the temperature-dependent trend in the shifts is clearly predictable from the distance and relative position of the proton from the Ce atom. Therefore, the Ce-encapsulated metallofullerene  $\text{Ce}@C_{82}$  can provide spatial location information about nearby atoms through the temperature-dependent paramagnetic shifts of its NMR signals. It can act as a molecular probe for location sensing by utilizing the anisotropic magnetism of the encapsulated Ce atom.

#### **Tuning of the photoluminescence and up-conversion photoluminescence properties of single-walled carbon nanotubes by chemical functionalization**

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*Nanoscale*, **8**, (2016) 16916–16921.

Alkylated single-walled carbon nanotubes (SWNTs) were synthesized by the reaction with alkyl bromide or alkyl dibromide, and the photoluminescence (PL) properties of the resulting alkylated SWNTs were characterized. Two new PL peaks were observed along with the intrinsic PL peak at 976 nm when alkyl bromide was used (SWNT-Bu: ~1095 and 1230 nm, SWNT-Bn: 1104 and 1197 nm). In contrast, the use of  $\alpha,\alpha'$ -dibromo-o-xylene as an alkyl dibromide primarily resulted in only one new PL peak, which was observed at 1231 nm. The results revealed that the Stokes shift of the new peaks was strongly influenced by the addition patterns of the substituents. In addition, the time-resolved PL decay profiles of the alkylated SWNTs revealed that the PL peaks possessing a larger Stokes shift had longer exciton lifetimes. The up-conversion PL intensity of the alkylated SWNTs at excitation wavelengths of 1100 and 1250 nm was estimated to be ~2.38 and ~2.35 times higher than that of the as-dispersed SWNTs, respectively.

### **Thermal Stability of Oxidized Single-Walled Carbon Nanotubes: Competitive Elimination and Decomposition Reaction Depending on the Degree of Functionalization**

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The thermal stability of oxidized single-walled carbon nanotubes (SWNTs) with various degrees of oxidation was investigated. The lower absorption and radial breathing mode (RBM) peaks and a higher intensity ratio of the D band to the G band (D/G) in their absorption and Raman spectra of oxidized SWNTs changed from those of the pristine SWNTs. After the thermal treatment, the D/G ratio of the oxidized SWNTs almost recovered its original intensity, regardless of the degree of oxidation. The absorption, photoluminescence (PL), and RBM peaks could not recover their original intensities when the oxidation degree was high. The results indicate that the elimination and decomposition reactions proceeded competitively depending on the degree of oxidation. In addition, a new PL peak was observed in the near-infrared region, and the PL peak intensity increased with the subsequent thermal treatment. The theoretical calculations provided an insight into the possible pathways for the decomposition of oxidized SWNTs, showing that the O<sub>2</sub> elimination and CO/CO<sub>2</sub> evolution proceed competitively during thermal treatment.

### **The Unanticipated Dimerization of Ce@C<sub>2v</sub>(9)-C<sub>82</sub> upon Co-crystallization with Ni(octaethylporphyrin) and Comparison with Monomeric M@C<sub>2v</sub>(9)-C<sub>82</sub> (M = La, Sc, and Y)**

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International Science Tsukuba)

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We report that  $\text{Ce}@C_{2v}(9)\text{-C}_{82}$  forms a centrosymmetric dimer in condition with single-crystal when co-crystallized with Ni(OEP) (OEP = octaethylporphyrin dianion). The crystal structure of  $\{\text{Ce}@C_{2v}(9)\text{-C}_{82}\}_2\cdot 2[\text{Ni}(\text{OEP})]\cdot 4\text{C}_6\text{H}_6$  shows that a new C-C bond with a bond length of 1.605(5) Å connects the two cages. On the other hand, the treatment of Ni(OEP) with  $\text{M}@C_{2v}(9)\text{-C}_{82}$  (M = La, Sc, and Y) results in crystallization of monomeric endohedral fullerenes. A systematic comparison of the X-ray structures of  $\text{M}@C_{2v}(9)\text{-C}_{82}$  (M = Sc, Y, La, Ce, Gd, Yb, and Sm) reveals that the major metal site in each case is located at an off-center position adjacent to a hexagonal ring along the  $C_2$  axis of the  $C_{2v}(9)\text{-C}_{82}$  cage. These results are supported by DFT calculations at the M06-2X level.

### **$D_{2d}(23)\text{-C}_{84}$ versus $\text{Sc}_2\text{C}_2@D_{2d}(23)\text{-C}_{84}$ : Impact of Endohedral $\text{Sc}_2\text{C}_2$ Doping on Chemical Reactivity in the Photolysis of Diazirine**

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We compared the chemical reactivity of  $D_{2d}(23)\text{-C}_{84}$  and that of  $\text{Sc}_2\text{C}_2@D_{2d}(23)\text{-C}_{84}$ , both having the same carbon cage geometry, in the photolysis of 2-adamantane-2,3'-[3H]-diazirine, to clarify metal-atom doping effects on the chemical reactivity of the carbon cage. Experimental and computational studies have revealed that the chemical reactivity of the  $D_{2d}(23)\text{-C}_{84}$  carbon cage is altered drastically by endohedral  $\text{Sc}_2\text{C}_2$  doping. The reaction of empty  $D_{2d}(23)\text{-C}_{84}$  with the diazirine under photoirradiation yields two adamantylidene (Ad) adducts. The major Ad monoadduct ( $\text{C}_{84}(\text{Ad})\text{-A}$ ) has a fulleroid structure and that the minor Ad monoadduct ( $\text{C}_{84}(\text{Ad})\text{-B}$ ) has a methanofullerene structure, which are identified by NMR spectroscopic studies. The latter was also determined by single-crystal X-ray crystallography.  $\text{C}_{84}(\text{Ad})\text{-A}$  is stable under photoirradiation, but it interconverted to  $\text{C}_{84}(\text{Ad})\text{-B}$  by heating at 80 °C. In contrast, four  $\text{Sc}_2\text{C}_2@D_{2d}(23)\text{-C}_{84}(\text{Ad})$  monoadducts were obtained by the reaction with diazirine under photoirradiation. The structure of  $\text{Sc}_2\text{C}_2@C_{84}(\text{Ad})\text{-C}$  was determined by single-crystal X-ray crystallography. Thermal interconversion of  $\text{Sc}_2\text{C}_2@C_{84}(\text{Ad})\text{-A}$  and  $\text{Sc}_2\text{C}_2@$

$C_{84}(\text{Ad})\text{-B}$  to  $\text{Sc}_2\text{C}_2@C_{84}(\text{Ad})\text{-C}$  was also observed. The reaction mechanisms of the Ad addition and thermal interconversion were elucidated from theoretical calculations. Calculation results suggest that  $C_{84}(\text{Ad})\text{-B}$  and  $\text{Sc}_2\text{C}_2@C_{84}(\text{Ad})\text{-C}$  are thermodynamically favorable products. Their different chemical reactivities derive from  $\text{Sc}_2\text{C}_2$  doping, which raises the HOMO and LUMO levels of the  $D_{2d}(23)\text{-C}_{84}$  carbon cage.

### Synthesis and Photoinduced Electron-Transfer Reactions in a $\text{La}_2@I_h\text{-C}_{80}$ -Phenoxazine Conjugate

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[http://libir.josai.ac.jp/il/meta\\_pub/G0000284repository\\_JOS-cplu.201600391](http://libir.josai.ac.jp/il/meta_pub/G0000284repository_JOS-cplu.201600391)

A newly designed electron donor-acceptor conjugated molecule consisting of an endohedral dimetallofullerene ( $\text{La}_2@I_h\text{-C}_{80}$ ) and phenoxazine (POZ) was successfully synthesized using Prato conditions. Our results show that the 1,3-dipolar cycloaddition took place across the [5,6] junction to afford exclusively the corresponding [5,6] cycloadduct. The structure of the conjugated molecule was characterized by  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopy, absorption spectroscopy, and electrochemical studies. Computational calculations suggest that the electron density of the highest occupied molecular orbital (HOMO) is distributed on the POZ moiety, whereas that of the lowest unoccupied molecular orbital (LUMO) is located at the endohedral La atoms, leading to efficient separation of the HOMO and LUMO in the conjugate. Time-resolved absorption spectroscopic investigations and spectroelectrochemical measurements corroborate the formation of the energetically low-lying  $(\text{La}_2@I_h\text{-C}_{80})^- (\text{POZ})^+$  radical-ion-pair state by means of ultrafast through-space electron transfer.

### Effect of Substituents and Initial Degree of Functionalization of Alkylated Single-Walled Carbon Nanotubes on Their Thermal Stability and Photoluminescence Properties

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[http://libir.josai.ac.jp/il/meta\\_pub/G0000284repository\\_JOS-chem.201604282](http://libir.josai.ac.jp/il/meta_pub/G0000284repository_JOS-chem.201604282)

Alkylated single-walled carbon nanotubes (SWNTs) have been thermally treated to determine the influence of substituents and the degree of functionalization on their thermal stability and photoluminescence (PL) properties. Alkylated SWNTs were synthesized by reaction of SWNTs with sodium naphthalenide and alkyl bromide. The defunctionalization of the alkylated SWNTs was monitored by absorption and Raman spectra. Selective recovery of the characteristic absorption and radial breathing mode peaks was observed during the thermal treatment, which indicates that the thermal stability of the alkylated SWNTs decreases with increases in SWNT diameter and degree of functionalization. n-Butylated and phenethylated SWNTs showed higher thermal stability than sec-butylated and benzylated SWNTs for a similar degree of functionalization, respectively. The diameter selectivity and effect of substituents on the thermal elimination reaction were confirmed by density functional theory. In addition, it was shown that the initial degree of functionalization of the alkylated SWNTs, with the alkyl group and degree of functionalization being kept constant after thermal treatment, strongly affects their PL properties; Stokes shift, and PL peak intensity.

### **Adamantylidene Addition to $M_3N@I_h-C_{80}$ (M=Sc, Lu) and $Sc_3N@D_{5h}-C_{80}$ : Synthesis and Crystallographic Characterization of the [5,6]-Open and [6,6]-Open Adducts**

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[http://libir.josai.ac.jp/il/meta\\_pub/G0000284repository\\_JOS-chem.201700049](http://libir.josai.ac.jp/il/meta_pub/G0000284repository_JOS-chem.201700049)

$M_3N@I_h-C_{80}$  (M = Sc, Lu) and  $Sc_3N@D_{5h}-C_{80}$  derivatives having Adamantyl group (Ad) have been synthesized by photochemical reactions with 2-adamantyl-2,3'-[3H]-diazirine. In  $M_3N@I_h-C_{80}$ , the addition led to rupture of the [6,6]- or [5,6]-bonds of the  $I_h-C_{80}$  cage, forming the [6,6]-open fulleroid as the major isomer and the [5,6]-open fulleroid as the minor isomer.

In  $\text{Sc}_3\text{N}@D_{5h}\text{-C}_{80}$ , the addition also proceeded regioselectively to yield three major isomeric Ad mono-adducts, despite the fact that there are nine types of C–C bonds in the  $D_{5h}\text{-C}_{80}$  cage. The molecular structures of the seven Ad mono-adducts, including the positions of the encaged trimetallic nitride clusters, have been unambiguously determined through single-crystal XRD analyses. Furthermore, results have shown that stepwise addition of Ad to  $\text{Lu}_3\text{N}@I_h\text{-C}_{80}$  affords several Ad bis-adducts, two of which have been isolated. The structure of one bis-adduct was characterized by single-crystal XRD analysis. The X-ray structure of one bis-adduct clearly revealed that the second Ad addition took place at a [6,6]-bond close to an endohedral metal atom. Theoretical calculations have also been performed to rationalize the regioselectivity.

### Temperature Dependence of Anisotropic Transient Conductivity of a $\text{La}@C_{2v}\text{-C}_{82}(\text{Ad})$ Crystal

Michio Yamada<sup>\*1</sup>, Satoru Sato<sup>\*2</sup>, Wookjin Choi<sup>\*3</sup>, Shu Seki<sup>\*3</sup>, Tsuneyuki Abe<sup>\*2</sup>, Mitsuaki Suzuki<sup>\*1,4</sup>, Yutaka Maeda<sup>\*1</sup>, Shigeru Nagase<sup>\*5</sup>, Takeshi Akasaka<sup>\*1,2,6,7</sup> (\*1 Department of Chemistry, Tokyo Gakugei University, \*2 Life Science Center of Tsukuba Advanced Research Alliance, University of Tsukuba, \*3 Department of Molecular Engineering, Kyoto University, \*4 Department of Chemistry, Josai University, \*5 Fukui Institute for Fundamental Chemistry, Kyoto University, \*6 Foundation for Advancement of International Science, \*7 State Key Laboratory of Materials Processing and Die and Mold Technology School of Materials Science and Engineering, Huazhong University of Science and Technology) *Chem. Lett.* **46**, 973–975.

The temperature dependence of the anisotropic transient conductivity of a  $\text{La}@C_{2v}(9)\text{-C}_{82}$  adamantyl derivative crystal was measured using flash-photolysis time-resolved microwave conductivity (FP-TRMC) measurements. Results showed that the transient conductivity along the c-axis of the single-crystal increased as the temperature decreased, proving that electron transport can be described by the electronic band-conduction model instead of the electron-hopping model.

### Activity Variation in Acid Phosphatase (ACPH) Allozymes of *Drosophila virilis* Resulting from Two Different *AcpH* Gene Transcripts

H. Kitagawa

*Drosophila Information Service* 98, 28–34 (December 2015)

To reveal the mechanism underlying ACPH allozyme activity variation in *D. virilis*, the acid phosphatase allelic genes *AcpH-1*, *AcpH-2*, and *AcpH-4* and their transcripts were isolated and characterized. Each gene includes six exons. Two major transcripts are formed by alternative splicing of exon 5, with two proteins of differing lengths produced as a consequence. Because exon 6 encodes a transmembrane segment, the long protein was inferred to be the membrane-bound form and the short protein the soluble one. Semi-quantitative and quantita-

tive real-time PCR analyses of these transcripts revealed that the membrane-bound protein had similar expression levels among the three allelic genes. In contrast, the soluble protein showed variable expression: levels of *Acph-4*, *Acph-2*, and *Acph-1* were high, medium, and low, respectively, with their expression ratio (4.6:3.1:1) corresponding approximately to relative enzyme activities observed by gel electrophoresis. Comparative analysis of *Acph* nucleotide sequences of *D. virilis* and related species revealed that the activity differences are not due to variation in active sites, disulfide bonds, or glycosylation sites.

### 城西大学におけるスチューデント・インターンシップ事業への取り組み

北川浩子

城西大学 教職センター紀要. **1**, 45-54 (11月 2017)

城西大学では女子栄養大学とともに坂戸市及び坂戸市教育委員会の協力のもと、平成18年度より「坂戸市スチューデント・インターンシップ事業」を通して坂戸市内の小・中学校へ学生を派遣している。この事業における取組みや実施体制を示し、平成18年度から5年間の事業の運営状況と理学部における学生の活動状況について報告する。そのアンケート結果からは多くの学生が教育実習や教員になることへの不安が解消され、自身の目標が明確になったことが示され、そしてそれが化学科においての教員採用試験での合格につながることを示唆された。

### Rapid and effective isolation of candidate sequences for development of microsatellite markers in 30 fish species facilitated by kit-based target capturing and massively multiplexed parallel sequencing

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Conservation Genetics Resources, **9**, 479-490 (2017)  
DOI: 10.1007/s12686-017-0699-z.

Recent advances in next-generation sequencing (NGS) technology have accelerated the development of microsatellite markers for wildlife conservation genetics. Although the discovery of microsatellite-containing sequences based on NGS is more efficient with sequencing of a microsatellite-enriched library than with wholegenome shotgun sequencing, the process of constructing a microsatellite-enriched library is somewhat complicated. Therefore, many researchers prefer to use external services for the microsatellite-enrichment, which requires more time. To facilitate the rapid and effective development of novel microsatellite markers, we attempted to simplify the process of constructing a microsatellite-enriched library for multiplexed parallel sequencing. To capture microsatellite-containing sequences, we applied an easy-to-use commercially available kit for the hybridization and wash steps. After preparing

shotgun libraries of 30 fish species for NGS, we captured microsatellite-containing DNA fragments directly from the shotgun libraries by using the commercially available kit. Next, three runs of multiplexed parallel sequencing were conducted on the 454 GS Junior platform. The resulting sequences for each species included high proportions of microsatellite-containing sequences (from 46 to 79%). Thus, sufficient numbers of primer sets, ranging from 1029 to 6606, were effectively designed for each species. Microsatellite capture and sequencing were completed in about a week, so the time required was substantially reduced. To validate the effectiveness of our strategy, we screened 44 potential primer sets designed for ayu (*Plecoglossus altivelis*). The results of polymorphisms revealed that allelic variability at 23 markers will be useful for studying population structure. These results prove the effectiveness of our improved approach for microsatellite marker development.

### **Localized phase separation of thermoresponsive polymers induced by plasmonic heating**

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*J. Phys. Chem. C*, **121**, 22496-22507 (2017).

Optical excitation-induced heating of a single gold nanoparticle potentially offers a high-temperature field confined to the immediate neighborhood of the particle. In this study, we applied darkfield microscopy imaging and Rayleigh scattering spectroscopy to pursue phase separation of aqueous thermoresponsive poly(*N*-isopropylacrylamide) and poly(vinyl methyl ether) adjacent to a gold nanoparticle that was heated by continuous wave laser illumination. Gold nanoparticles were supported on transparent substrates of glass or sapphire. From the imaging study, we observed that a 1-10  $\mu\text{m}$  microdroplet covering the nanoparticle formed and grew in time scales of seconds to a few tens of seconds. The growth was triggered by the illumination, and the droplet collapsed when the laser was blocked. At the same time, we observed scattering spectral changes characterized by a progressive redshift in the localized surface plasmon resonance (LSPR) band and an increasing scattering intensity in the region of wavelengths shorter than the LSPR band with increasing laser intensity. The scattering spectral changes were interpreted by the encapsulation of the nanoparticle by a polymer-rich droplet with increasing sizes. The present study revealed that thermoresponsive polymers were attracted to a hot gold nanoparticle and formed a microdroplet under illumination with a wavelength near the LSPR. Our findings demonstrate the potential of plasmonic heating to manipulate polymer migration and accumulation, which may find applications in protein crystallization.

### **Preparation and micropatterning of gold nanoparticles by femtosecond laser-induced optical breakdown**

Takayuki Uwada, Shun-Fa Wang\*, Tsung-Han Liu\*, Hiroshi Masuhara\* (\* Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Taiwan)



*J. Photochem. Photobiol. A*, **346**, 177-186 (2017).

We fabricated gold nanoparticles (NPs) via a femtosecond (fs) laser-induced cavitation bubbling. By introducing intense fs laser pulses into H<sub>2</sub>AuCl<sub>4</sub> aqueous solution containing 1-propanol, optical breakdown and the following cavitation bubble generation occurred at the focus through multiphoton absorption of water, resulting in the formation of gold nanoparticles (Au NPs). Intermediate species such as radicals and solvated electrons produced upon the bubbling contribute to gold ion reduction, while direct ionization of Au-chloride complex, photothermal decomposition and direct optical decomposition are excluded as possible mechanisms. Utilizing the fs laser-induced bubbling we demonstrate in-situ micropatterning of Au NPs on a substrate from the same H<sub>2</sub>AuCl<sub>4</sub> aqueous solution containing 1-propanol.

### **Size-dependent optical properties of grana inside chloroplast of plant cells**

Takayuki Uwada, Ling-Ting Huang<sup>\*1</sup>, Ping-Yu Hee<sup>\*1</sup>, Anwer Usman<sup>\*2</sup>, Hiroshi Masuhara<sup>\*1</sup> (\*1 Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Taiwan, \*2 Department of Chemistry, Faculty of Science, Universiti Brunei Darussalam, Negara Brunei Darussalam)  
*J. Phys. Chem. B*, **121**, 915-922 (2017).

Well-packed thylakoids known as grana are one of the major functional sites for photosynthesis in algae and plants. Their highly ordered structures can be considered as a few hundred nanometer-sized particles having distinct scattering cross sections from other various macromolecular organizations inside plant cells. With this background we show that elastic light scattering imaging and microspectroscopy is an important tool for investigating structure and organization of grana inside a single chloroplast in plant cells. We have demonstrated this noninvasive method to identify the distribution of grana in intact fresh leaf of robust and rapidly growing *Egeria densa*, which is also known as Anachris and among the most popular aquarium plants. The scattering efficiency spectra of their individual grana fairly resemble cooperative absorption spectra of porphyrins and carotenoids. We found that the electronic structure of the stacked thylakoids shows granum size-dependence, indicating that size of grana is one of the critical parameters in the regulation of the photochemical functions in the thylakoid.

### **Laser-driven phase transitions in aqueous colloidal gold nanoparticles under high pressure: picosecond pump-probe study**

Shuichi Hashimoto<sup>\*1</sup>, Tetsuro Katayama<sup>\*2</sup>, Kenji Setoura<sup>\*2</sup>, Michael Strasser<sup>\*1</sup>, Takayuki Uwada, Hiroshi Miyasaka<sup>\*2</sup> (\*1 Department of Optical Science and Technology, University of Tokushima, \*2 Division of Frontier Materials Science, Osaka University)  
*Phys. Chem. Chem. Phys.*, **18**, 4994-5004 (2016).

Pump-probe transient extinction spectroscopy was used to analyze 355 nm picosecond laser heating-induced phenomena in 60 nm-diameter aqueous gold nanoparticles (AuNPs) under a high pressure of 60 MPa. Kinetic spectroscopy revealed that a supercritical layer surrounding the AuNP nucleated with a lifetime of approximately 1 ns during its dynamic expansion and decay for a fluence of  $19.6 \text{ mJ cm}^{-2}$ . Moreover, in the post-mortem transmission electron micrographs we observed a number of fragments, a small percentage of size-reduced cores, and erupted particles among the intact particles after 60 shots, suggesting that evaporation occurred under laser illumination. The particle temperature calculation indicated that evaporation begins with a liquid droplet AuNP surrounded by a supercritical layer at temperatures below the boiling point of gold. By applying high pressure, we obtained a clear picture of the evaporation event, which was not possible at ambient pressure because bubble formation caused particle temperatures to rise uncontrollably. In this study, we shed light on the critical role of the supercritical layer formed around the AuNP under high pressure during laser-induced evaporation.

### **Plasmonic nanofabrication through optical heating**

Matthias Enders\*, Shinya Mukai\*, Takayuki Uwada, and Shuichi Hashimoto\* (\* Department of Optical Science and Technology, University of Tokushima)  
*J. Phys. Chem. C*, **120**, 6723-6732 (2016).

A temperature gradient can induce solutes to migrate from a hot to a cold region, and vice versa, in solution. This process, termed thermophoresis, has been applied to manipulate, transport, and separate various macromolecules and colloids by exploiting a microscale temperature gradient. Here we describe using a single gold nanoparticle (AuNP) as an efficient nanoscale heating source to promote thermophoresis. Moreover, on introducing a substrate with high thermal conductivity such as sapphire, a strong local temperature gradient can be shaped in the medium near the AuNP under continuous wave laser illumination. We observed molecules such as polyethylene glycol and sodium dodecyl sulfate being transported toward the AuNP and attaching to its surface, forming a gold core-organic shell structure within several tens of seconds of illumination. Spectroscopically, because of the gradual increasing encapsulation, progressive red shifts with enhanced scattering intensities were seen for the localized surface plasmon resonance bands of the AuNP with increasing cycles of illumination. Post-mortem scanning electron microscopy provided direct evidence of shell formation. Our technique is relevant to nanofabrication based upon optical heating at the nanometer scale.

### **Enhancement of Cytotoxicity of Three Apoptosis-inducing Agents Against Human Oral Squamous Cell Carcinoma Cell Line by Benzoxazinotropone**

Yukiko Tomikoshi, Maki Nomura, Noriyuki Okudaira,\*<sup>1</sup> Hiroshi Sakagami,\*<sup>1</sup> and Hidetsugu Wakabayashi (\*<sup>1</sup> Department of Endodontics, Meikai University School of Dentistry)  
*International Journal of In Vivo Research*, **30**, 645-650 (2016).

Tumor-specificity (TS) and anti-inflammatory activity of benzo[*b*]cyclohept[*e*][1,4]oxazin-6(11*H*)-one, generally known as benzoxazinotropone (BOT), have been reported. In order to find a new biological activity, the combination effect of BOT and three apoptosis-inducing agents was investigated. Cytotoxicity against four human oral squamous cell carcinoma (OSCC) cell lines and five human oral normal cells (gingival fibroblasts, periodontal ligament fibroblasts, pulp cells, oral keratinocytes and primary gingival epithelial cells) was determined by 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) method. TS was evaluated by the ratio of the mean 50% cytotoxic concentration (CC<sub>50</sub>) against normal oral cells to the one against OSCC cell lines. Expression of cleaved forms of poly ADP-ribose polymerase and caspase-3 was evaluated by western blot analysis. BOT induced activation of caspase 3, suggesting the apoptosis induction in HSC-2 OSCC cells. BOT enhanced the cytotoxicity of doxorubicin (DXR) additively and that of curcumin and resveratrol synergistically. On the other hand, BOT did not enhance, but rather inhibit the cytotoxicity of DXR against normal keratinocytes. The present study suggests that BOT may enhance the anti-tumor activity of apoptosis-inducing agents, while reducing its cytotoxicity against normal cells.

#### **Photoluminescence properties of TADF-emitting three-coordinate silver(I) halide complexes with diphosphine ligands: a comparison study with copper(I) complexes**

Masahisa Osawa<sup>\*1,2</sup>, Masashi Hashimoto, Isao Kawata<sup>\*2</sup> and Mikio Hoshino<sup>\*2</sup>

(\*1 Luminescent Materials Laboratory, \*2 Department of Applied Chemistry, Nippon Institute of Technology)

*Dalton Trans.*, **46**, 12446-12455 (2017).

Synthesis of silver(I) bromide complexes with diphosphine ligands LMe, LEt, and LiPr are described. Crystals of complex [(LMe)AgBr]<sub>2</sub>, prepared from LMe and AgBr, showed a tetrahedral bimetallic structure. LEt and LiPr, with bulkier substituents than those of LMe, reacted with AgBr to give crystalline three-coordinate complexes (LEt)AgBr and (LiPr)AgBr. Nuclear magnetic resonance (NMR) studies demonstrated that [(LMe)AgBr]<sub>2</sub> dissociates in solution to yield a monomeric three-coordinate complex (LMe)AgBr.

#### **Novel synthesis of 1,2-dihydro-4*H*-3,1-benzoxazine-4-thiones by the reaction of newly synthesized methyl dithioanthranilate hydrobromide with carbonyl compounds and synthesis of another new class of 1,2-dihydro-4*H*-3,1-benzothiazine-4-thiones from the same reactants in the presence of excess sodium hydrosulfide**

Tatsuo Yamamoto and Motomu Muraoka

*Heterocycl* **91**, 2327-2342 (2015)

Methyl dithioanthranilate hydrobromide (**6**) was synthesized by deprotection of Z-protected methyl dithioanthranilate (**5**) which was obtained by treatment of Z-protected methylthioiminium iodide **4** with H<sub>2</sub>S. 1,2-Dihydro-4*H*-3,1-benzoxazine-4-thiones **10a-m** were

first synthesized by the reaction of methyl dithioanthranilate hydrobromide (**6**) and each aldehyde or ketone. Formaldehyde, in this reaction, gave *N*-(methylthio)methyl-4*H*-3,1-benzoxazine-4-thione (**11**). Another new class of 1,2-dihydro-4*H*-3,1-benzothiazine- 4-thiones **12a-e** were synthesized from the same reactants in the presence of two equivalents of sodium hydrogensulfide.

#### 簡易な器具を用いた水の電気分解によるアボガドロ数の決定実験の教材化

山本達夫

城西大学教養課程センター紀要創刊号, 71-74, (2017)

安価な自作および汎用器具と乾池を用いた簡易電気分解装置を用い、アボガドロ数を測定できる実験を考案した。本考案装置を教材として用いて、本学化学科1年生の化学実験において27年間用いてきた結果をまとめ、報告する。学生が出したアボガドロ数は誤差±3.6%以内に収まっており、本実験は大学初等教育のファラデー定数、アボガドロ数、電気分解の概念を修得する化学実験として優れた教材である。

## 2. Books, Reviews and Other Printings

### MATHEMATICS

#### **Riemann 球面上の複素常微分方程式と多変数超幾何関数**

大島利雄

第 14 回岡シンポジウム講演集, 53-97, 2016.

#### **数学諸分野における線形代数**

大島利雄

特集:「線形代数の探究」, 数理科学 8 月号, 638 (2016), 22-28.

#### **【特別講演】数式処理による線型代数や微積分の問題と解法**

大島利雄

数学ソフトウェアとその効果的教育利用に関する研究, 数理解析研究所講究録 2022 (2017), 1-9.

#### **KZ 型超幾何系の変換と解析**

大島利雄

表現論と非可換調和解析をめぐる諸問題, 数理解析研究所講究録 2031 (2017), 124-158.

#### **ベジェ曲線による曲線近似とその応用**

大島利雄

数式処理とその周辺分野の研究, 数理解析研究所講究録 2054 (2017), 96-104.

#### **第 56 回実関数論・関数解析合同シンポジウム講演集 (2017)**

<http://mathsoc.jp/~section/~fctanalysis/~Proceedings2017.pdf>

#### **研究集会「結び目の数学 X」報告集 (2017)**

<http://www.math.twcu.ac.jp/~mok10procn/~13Kogiso.pdf>

#### **英国の古くから知られる童謡に見られるある数理現象と, その教材としての教育効果について**

<http://libir.josai.ac.jp/~il/~metapub/~G0000284repositoryJOS-sugakukyoshoku-1031> 教職課程用講義・実践編

#### **朝倉 数学辞典 (変換群の部分 執筆)**

神島芳宣

朝倉書店, 2016 年

## CHEMISTRY

### **Plant-microbe-metal Interactions: Basics, Recent Advances and Future Trends**

Shelake R. M., Waghunde R. R., Morita E. H., Hayashi, H.

*Plant Microbiome: Stress Response* ed Egamberdieva D. and Ahmad P. (Springer Nature Singapore Pte Ltd.) pp. 283-305 (2017)

### **福井県越前市域におけるドジョウ (*Misgurnus anguillicaudatus*) の遺伝的特性**

日和佳政<sup>\*1</sup>, 藤長裕平<sup>\*1</sup>, 高橋将人, 石黒直哉 (\*1 越前市産業環境部)

DNA 多型, **25**, 30-35 (2017).

### **淡水エビ分布調査を目的とした環境 DNA 分析手法の開発**

石黒直哉, 飯島大智, 石田季久

DNA 多型, **25**, 85-87 (2017).

### **高分解能光学顕微鏡**

石川 満

光と生命の事典, 日本光生物学協会, 光と生命の事典編集委員会編 pp. 384-385 朝倉書店 (2016)

### **ナトリウムアルコキシドとフラノン類からなる 2 成分オイルゲル化剤の開発**

橋本雅司

月間ファインケミカル, **45** (10), 12-19 (2016).

### 3. Oral Presentations

#### MATHEMATICS

##### First order differential equations

T. Oshima

*International Conference of Partial Differential Equations: General Theory and Variational Problems*, フィリピン, Cebu, Jan. 14, 2016.

##### TEX/ 数式処理による教材作成

奥村晴彦, 大島利雄, 高橋 正, 高遠節夫

パネルディスカッション, 日本数式処理学会合同分科会, 名古屋大学, Jan. 23, 2016.

##### Differential equations related to Whittaker functions and moderate growth

T. Oshima

International Conference : Geometry, Representation Theory and Differential Equations, 九州大学 IMI Auditorium, Feb. 18, 2016.

##### TEX 描画と描画データの数学的処理との有機的連携

金子真隆, 大島利雄, 高遠節夫

日本数学会年会, 応用数学, 筑波大学, Mar. 16, 2016.

##### 多変数超幾何微分方程式の可約性について

アクセサリー・パラメータ研究会, 熊本大学, Mar. 22, 2016.

##### Risa/Asir を用いた積分や行列の問題とその計算

大島利雄

数式処理とその教育利用, 東京理科大学神楽坂キャンパス, May 14, 2016.

##### KZ 型超幾何系の変換と解析

大島利雄

表現論と非可換調和解析をめぐる諸問題, 京都大学数理解析研究所, June 30, 2016.

##### 数式処理の数学教育への活用

大島利雄

幾何学とインターネットの数理 2016, 東京大学玉原国際セミナーハウス, July 17, 2016.

##### KZ 型方程式の middle convolution

大島利雄

2016 年度函数方程式論サマーセミナー, いこいの村能登半島, Aug. 2, 2016.

**KZ 型超幾何微分方程式の middle convolution について**

大島利雄

アクセサリー・パラメータ研究会, 東京大学玉原国際セミナーハウス, Aug. 24, 2016.

**数学教育における数式処理と T<sub>E</sub>X の活用**

大島利雄

数学ソフトウェアとフリードキュメント XXIII, 関西大学, Sep. 14, 2016.

**数式処理による線型代数や微積分の問題と解法の作成**

大島利雄

数学ソフトウェアとその効果的教育利用に関する研究, 京都大学数理解析研究所, Sep. 29, 2016.

**正則パラメータの完備化とそのアルゴリズム**

大島利雄

数式処理とその周辺分野の研究, 京都大学数理解析研究所, Dec. 8, 2016.

**KZ 型方程式の解析**

大島利雄

超幾何方程式研究会 2017, 神戸大学, Jan. 6, 2017.

**KZ 型方程式の変換と完全積分可能条件**

大島利雄

2016 年度表現論ワークショップ, 鳥取県民ふれあい会館, Jan. 8, 2017.

**リジッドな Fuchs 型方程式の半局所モノドロミー**

大島利雄

可積分系ウインターセミナー 2017, 越後湯沢, Feb. 4, 2017.

**リジッドなフックス型方程式の semilocal monodromy や KZ 型方程式のスペクトル型の計算**

大島利雄

アクセサリー・パラメータ研究会, 熊本大学, Mar. 16, 2017.

**Risa/Asir における積分計算**

大島利雄

Risa/Asir Conference 2017, 金沢大学, Mar. 29, 2017.

**Rigid Fuchsian ordinary differential equations and equations of KZ-type**

T. Oshima

Algebraic Analysis and Representation Theory, 京都大学数理解析研究所, Jun. 29, 2017.

**計算尺を使った教育**

大島利雄



幾何学とインターネットの数理 2017, 東京大学玉原国際セミナーハウス, Jul. 16, 2017.

### 計算尺の教育への活用

大島利雄

数学ソフトウェアとその効果的教育利用に関する研究, 京都大学数理解析研究所, Aug. 31, 2017.

### Rigid Fuchsian ordinary differential equations and equations of KZ-type

T. Oshima

Formal and Analytic Solutions of Diff. Equations 2017, Alcalá de Henares, Spain, Sep. 7, 2017.

### 計算尺を使った教育

大島利雄

アクセサリー・パラメータ研究会, 東京大学玉原国際セミナーハウス, Oct. 6, 2017.

### KZ 方程式や rigid Fuchs 系における middle convolution などの変換

大島利雄

アクセサリー・パラメータ研究会, 東京大学玉原国際セミナーハウス, Oct. 9, 2017.

### Transformations of KZ type equations

大島利雄

超局所解析と漸近解析, 京都大学数理解析研究所, Oct. 19, 2017.

### 超幾何微分方程式の変換とその計算

大島利雄

複素微分方程式の楽しみ, 熊本大学, Nov. 3, 2017.

### Risa/Asir と他のプログラムの連携

大島利雄

数式処理とその周辺分野の研究, 京都大学数理科学研究所, Dec. 21, 2017.

### ある種の generic catalecticant の Legendre 変換と b-関数

小木曾岳義

表現論ワークショップ, ふれあい会館生涯学習センター, 鳥取市, 2016年1月10日

### Local functional equations of non-prehomogeneous type

Takeyoshi Kogiso

International conference "Geometry, Representation Theory, and Differential Equations"

Kyushu University, Ito campus, 九州大学 IMI, 2016年2月16日

### 極化の概均質性の遺伝と, 極化の関数等式

小木曾岳義

概均質ベクトル空間の分類研究とその周辺セミナー, 秋田大学教育文化学部, 2016年8月24日

**極化の概均質性の遺伝と，極化の関数等式**

小木曾岳義

概均質セミナー，早稲田大学教育学部，14号館，2016年10月22日

**Local functional equations associated to the polarization of homaloidal polynomials**

Takeyoshi Kogiso

JMM workshop, 城西大学紀尾井町キャンパス5号館，2016年11月26日

**Unimodular 群に関する Lagrange の定理のある種の証明とマルコフ数との関係**

小木曾岳義

表現論ワークショップ，ふれあい会館生涯学習センター，鳥取市，2017年1月8日

**Local functional equations associated with polarizations of homaloidal polynomials**

Takeyoshi Kogiso

Meeting for Study of Number theory, Hopf algebras and related topics, 富山大学理学部 B121,

2017年2月14日

 **$SL(2, \mathbb{Z})$ -diamonds のいくつかの応用について**

小木曾岳義

さきがけ研究集会「行列解析とその周辺」, 名古屋大学多元数理科学研究科，2017年3月30日

**Homaloidal 多項式の極化に付随する局所関数等式**

小木曾岳義

第56回実関数論・関数解析合同シンポジウム，お茶の水女子大学，2017年8月22日

**3次元概均質ベクトル空間の裏返し変換から得られる結び目多項式とその応用**

小木曾岳義

研究集会「概均質ベクトル空間の分類とその周辺」, 秋田大学教育学部，2017年8月24日

**Kauffman bracket polynomials of Conway Coxeter Friezes**

小木曾岳義

研究集会「結び目の数学 X」, 東京女子大学，2017年12月24日

**Security evaluation of a finger vein authentication algorithm against wolf attack**

Akira Otsuka, Tetsushi Ohki, Ryogo Morita, Manabu Inuma, Hideki Imai

37th IEEE Symposium on Security and Privacy, San Jose, CA, May 23, 2016

**PRACTICE における情報共有基盤の構築**

畑 太一, 井沼 学, 四方順司, 今村 祐, 竹内 新

2016年度電子情報通信学会総合大会，九州大学（伊都キャンパス），Mar. 18, 2016.

**Autonomous limit of the 4-dimensional Painlevé-type equations and degeneration of curves of genus two**

中村あかね

応用解析研究会, 天満研修センター, 2016年5月20日.

**Autonomous limit of the 4-dimensional Painlevé-type equations and degeneration of curves of genus two**

中村あかね

SIDE 12, Sainte-Adèle, Québec, カナダ, 2016年7月8日.

**Autonomous limit of the 4-dimensional Painlevé-type equations and degeneration of the Liouville tori**

中村あかね

函数方程式論サマーセミナー, いこいの村能登半島, 2016年8月5日.

**Isospectral limit of the Painlevé-type equations and degeneration of curves**

中村あかね

OCAMI Meeting on Integrable Systems, Moduli Spaces and Non-linear PDE, 大阪市立大学, 2016年9月3日.

**Isospectral limit of the Painlevé-type equations and degeneration of curves**

中村あかね

Painlevé equations and discrete dynamics, Banff International Research Station, カナダ, 2016年10月6日.

**Isospectral limit of the Painlevé-type equations and degeneration of curves**

中村あかね

青山数理セミナー, 青山学院大学, 2016年11月4日.

**Isospectral limit of the Painlevé-type equations and degeneration of curves**

中村あかね

The First Japan-Taiwan Joint Conference on Differential Geometry and the 8th TIMS-OCAMI-WASEDA Joint International Workshop on Differential Geometry and Geometric Analysis, 早稲田大学, 2016年12月16日.

**Three incarnation of the theta divisor of the Liouville tori**

中村あかね

離散数理モデリングセミナー, 東京大学, 2016年12月17日.

**Three incarnations of the theta divisor of the Liouville tori**

中村あかね

可積分系ウィンターセミナー, 越後湯沢KKR雪国, 2017年2月4日.

**Two incarnations of the theta divisor of the Liouville tori**

中村あかね

複素領域における関数方程式とその周辺, 広島大学, 2017年3月7日.

**Two incarnations of the theta divisor of the Liouville tori**

中村あかね

The Tenth IMACS International Conference on Nonlinear Evolution Equations and Wave, Georgia Center for Continuing Education University of Georgia, USA, 2017年3月30日.

**The 4-dimensional Painlevé-type equations and degeneration of genus two**

中村あかね

ISQS 25, The XXVth International Conference on Integrable Systems and Quantum symmetries, チェコ工科大学, 2017年6月8日.

**4次元パンルヴェ型方程式と種数2曲線の退化**

中村あかね

微分方程式と幾何学, 立命館大学, 2017年6月14日.

**The Painlevé equations revisited**

中村あかね

応用可積分系若手セミナー, 武蔵野大学, 2017年9月9日.

**確率微分方程式のスパース推定について**

清水優祐

2017年JMMワークショップ, 城西大学, 2017年11月.

## CHEMISTRY

### **Hamiltonian algorithm and its application to the aromatic oxidative cyclization on *N*-methoxy-*N*-prenylbenzamide**

Hiroyuki Teramae, Kousuke Hayashi<sup>\*1</sup>, Jun Takayama<sup>\*1</sup>, Takeshi Sakamoto<sup>\*1</sup> (\*1 Faculty of Pharmaceutical Sciences, Josai University)

ICCMSE 2016 (Athens), 2016 年 3 月, CC Symposium Materials (6), Organics, Excited State (invited)

### **2-アザスピロ環化合物の安定構造の理論的研究**

寺前裕之, 須田 岬, 林 浩輔<sup>\*1</sup>, 高山 淳<sup>\*1</sup>, 坂本武史<sup>\*1</sup> (\*1 城西大薬)

日本コンピュータ化学会 2016 年春季年会 (東京), 2016 年 5 月, 講演要旨集 1012

### **高次元アルゴリズムによる 2-アザスピロ環化合物の安定構造の理論的研究**

寺前裕之

第 4 回三重大学 CUTE シンポジウム (津), 2016 年 6 月, セッション 3 (招待講演)

### **Hamiltonian Algorithm Study of Aromatic Oxidative Cyclization on *N*-Methoxy-*N*-Prenylbenzamide**

Hiroyuki Teramae, Kousuke Hayashi<sup>\*1</sup>, Jun Takayama<sup>\*1</sup>, Takeshi Sakamoto<sup>\*1</sup> (\*1 Faculty of Pharmaceutical Sciences, Josai University)

12th European Conference on Atoms, Molecules and Photons (ECAMP12) (Frankfurt), 2016 年 9 月, Tue 113

### **2-アザスピロ環化合物の安定構造の理論的研究**

寺前裕之, 林 浩輔<sup>\*1</sup>, 高山 淳<sup>\*1</sup>, 坂本武史<sup>\*1</sup> (\*1 城西大薬)

分子科学討論会 2016 (神戸), 2016 年 9 月, 講演要旨集 2P105

### **2-アザスピロ環化合物における閉環反応の理論的研究**

寺前裕之, 林 浩輔<sup>\*1</sup>, 高山 淳<sup>\*1</sup>, 坂本武史<sup>\*1</sup> (\*1 城西大薬)

第 39 回ケモインフォマティクス討論会 (浜松), 2016 年 9 月, 講演要旨集 03

### **拡張基底関数依存性について**

平野恒夫<sup>\*1</sup>, 長嶋雲兵<sup>\*2</sup>, 寺前裕之, 長岡伸一<sup>\*3</sup> (\*1 お茶大, \*2 産総研, \*3 愛媛大)

日本コンピュータ化学会 2016 年秋季年会 (島根), 2016 年 10 月, 講演要旨集 1P03

### **結晶軌道法による DNA の Hartree-Fock 計算の試み**

寺前裕之, 青木百合子<sup>\*1</sup> (\*1 九大)

日本コンピュータ化学会 2016 年秋季年会 (島根), 2016 年 10 月, 講演要旨集 2007

### **Hamiltonian Algorithm Study of Aromatic Oxidative Cyclization on 2-Azaspiro Ring Compounds**

Hiroyuki Teramae, Kousuke Hayashi<sup>\*1</sup>, Jun Takayama<sup>\*1</sup>, Takeshi Sakamoto<sup>\*1</sup> (\*1 Faculty of Pharmaceutical Sciences, Josai University)

Stereodynamics 2016 (Taipei), 2016 年 11 月, Oral Presentation 8 (invited)

### **An Attempt at Ab Initio Crystal Orbital Calculation of Electronic Structure of B-type model-DNA**

Hiroyuki Teramae, Yuriko Aoki<sup>\*1</sup> (\*1 Kyushu University)

ICCMSE2017 (Thessaloniki), 2017 年 4 月, CC Symposium (7) Biology (invited)

### **フェルラ酸の抗酸化作用に関する理論的研究**

寺前裕之, 加藤洋介<sup>\*1</sup>, 高山 淳<sup>\*1</sup>, 坂本武史<sup>\*1</sup> (\*1 城西大薬)

日本コンピュータ化学会 2017 年春季年会 (東京), 2017 年 6 月, 講演要旨集 2P03

### **Ab initio crystal orbital calculation of electronic structure of B-type model-DNA**

Hiroyuki Teramae, Yuriko Aoki<sup>\*1</sup> (\*1 Kyushu University)

*11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2017)* (Munich), 2017 年 8 月, PO1-141

### **Ab initio calculations on polymononucleotide and polydinucleotides as model of B-type DNA polymers.**

Hiroyuki Teramae, Yuriko Aoki<sup>\*1</sup> (\*1 Kyushu University)

*11th European Conference on Theoretical and Computational Chemistry (EUCCO-TCC 2017)* (Barcelona), 2017 年 9 月, P71

### **モデル DNA の Hartree-Fock 計算**

寺前裕之, 青木百合子<sup>\*1</sup> (\*1 九大)

分子科学討論会 2017 (仙台), 2017 年 9 月, 講演要旨集 3F09

### **DNA の電子状態計算**

寺前裕之, 青木百合子<sup>\*1</sup> (\*1 九大)

日本コンピュータ化学会 2017 年秋季年会 (熊本), 2017 年 10 月, 講演要旨集 2003

### **フェルラ酸の抗酸化作用に関する理論的研究**

寺前裕之, 加藤洋介<sup>\*1</sup>, 高山 淳<sup>\*1</sup>, 坂本武史<sup>\*1</sup> (\*1 城西大薬)

第 40 回ケモインフォマティクス討論会 (山口), 2017 年 10 月, 講演要旨集 07

### **pyridine 溶媒中の pyrrole の NH 伸縮振動の基本音・倍音の吸収強度**

二見能資<sup>\*1</sup>, 尾崎 裕, 尾崎幸洋<sup>\*2</sup> (\*1 熊本高専, \*2 関西学院大)

第 10 回分子科学討論会 (神戸), 2016 年 9 月

**水素結合形成と NH 伸縮振動の倍音の吸収強度に関する考察**

二見能資<sup>\*1</sup>, 尾崎 裕, 尾崎幸洋<sup>\*2</sup> (\*1 熊本高専, \*2 関西学院大)  
平成 29 年度日本分光学会年次講演会 (東京), 2017 年 5 月

**水素結合形成と OH 伸縮振動の倍音の吸収強度に関する考察**

二見能資<sup>\*1</sup>, 尾崎 裕, 尾崎幸洋<sup>\*2</sup> (\*1 熊本高専, \*2 関西学院大)  
第 11 回分子科学討論会 (仙台), 2017 年 9 月

**Development of TiO<sub>2</sub> thin films aimed at high-efficient dye sensitized solar cells**

Takumu Fujiya, Akane Saito, Koichiro Mitsuke  
32nd Symposium on Chemical Kinetics and Dynamics (Saitama), 2016 年 6 月, Book of Abstracts, 1P16

**Transient photoluminescence spectroscopy of organic dyes adsorbed on thin films of metal oxide semiconductor**

Koichiro Mitsuke, Yo Tatsuno, Soshi Inaba  
32nd Symposium on Chemical Kinetics and Dynamics (Saitama), 2016 年 6 月, Book of Abstracts, 2P07

**Kinetics of electron injection from donor- $\pi$ -acceptor type dyes to nanocrystalline metal oxide semiconductors**

Takumu Fujiya, Nobuhide Tanaka, Koichiro Mitsuke, Katsuya Takahashi, Masashi Hashimoto  
32nd Symposium on Chemical Kinetics and Dynamics (Saitama), 2016 年 6 月, Book of Abstracts, 2P17

**Spectroscopies in millisecond and subnanosecond time-domains for DSSCs with new donor- $\pi$ -acceptor type organic dyes (invited)**

Koichiro Mitsuke  
Symposium on materials concepts for solar energy conversion and energy storage, Kasetsart University (Bangkok), 2016 年 8 月 26 日

**金属酸化物半導体薄膜に吸着したプッシュプル型有機色素の過渡発光分光**

渡邊晃平, 藤谷拓夢, 見附孝一郎, 高橋克弥, 橋本雅司  
2016 年光化学討論会 (東京) 2016 年 9 月, 講演予稿集, 3P-035

**Syntheses of ZnO nanorods on glass or flexible substrates utilized for manufacturing dye-sensitized solar cells**

Yuta Masuoka, Shinnosuke Hanayama, Tomoki Gomi, Tomotaka Naito, Koichiro Mitsuke  
33rd Symposium on Chemical Kinetics and Dynamics (Nagoya) 2017 年 6 月, Book of Abstracts, 1P13

**Design and construction of multilayer TiO<sub>2</sub> thin films used for photovoltaic electrodes**

Takumu Fujiya, Takuya Inuzuka, Koichiro Mitsuke

33rd Symposium on Chemical Kinetics and Dynamics (Nagoya) 2017年6月, Book of Abstracts, 1P05

**Transient emission spectroscopy of the D- $\pi$ -A type organic dyes adsorbed on metal oxide semiconductor nanoparticles**

Kouhei Watanabe, Akira Yoshida, Yo Tatsuno, Koichiro Mitsuke, Katsuya Takahashi, Masashi Hashimoto

33rd Symposium on Chemical Kinetics and Dynamics (Nagoya) 2017年6月, Book of Abstracts, 1P09

**金属酸化物半導体に吸着した D- $\pi$ -A 型色素分子の過渡発光分光**

渡邊晃平, 高柳康平, 吉田 輝, 見附孝一郎, 高橋克弥, 橋本雅司

2017年光化学討論会(仙台)2017年9月, 講演予稿集, 3P-19

**酸化亜鉛ナノロッドによる色素増感太陽電池のインピーダンス解析**

増岡優太, 渡井綾平, 見附孝一郎

第11回分子科学討論会(仙台)2017年9月, 講演要旨集, 3P-068

**色素増感太陽電池の陽極に用いる光反射層の作製と評価**

犬塚拓哉, 藤谷拓夢, 見附孝一郎

第11回分子科学討論会(仙台)2017年9月, 講演要旨集, 4P-064

**A novel mechanism of “metal gel-shift” by histidine-rich Ni<sup>2+</sup>-binding Hpn protein from *Helicobacter pylori* strain SS1**

Shelake, R.M., Ito, Y., Matsumoto, J., Morita, E.H., Hayashi H.

Gordon Research Conference (GRC) Metals in Biology, Ventura, CA, 93001, USA, Jan. 25, 2017

**Physicochemical studies for the heavy-metal stress response in cyanobacterium, *Synechococcus* sp. PCC 7942**

Eugene Hayato Morita, Shelake Rahul Mahadev, Kaneko Aibara, Hidenori Hayashi

5th International Symposium in Plant Signaling and Behavior, Matsue, June 30, 2017.

**Structural studies for small heat shock protein Orf7.5 in cyanobacterium *Synechococcus elongatus* PCC 7942**

E.H. Morita, N. Omiya, N.Ishikawa, H. Nakamoto, H. Hayashi

5th International Symposium in Plant Signaling and Behavior, Matsue, June 30, 2017.

**Structural studies of the cyanobacterial RNA-binding protein, RbpD, from *Anabaena variabilis***

Y. Tanaka, N. Sato, H. Hayashi, E.H. Morita



5th International Symposium in Plant Signaling and Behavior, Matsue, June 30, 2017.

**藍色細菌由来の低分子量熱ショックタンパク質 Orf 7.5 の構造機能相関**

森田勇人, 大宮永行, 石川奈都子, 田中直樹, 林 秀則, 仲本 準  
第 56 回 NMR 討論会, 首都大学東京, Nov. 16, 2017

**ヤエヤマサソリ由来毒素 LaIT2 の構造機能相関解析**

田村真生, 十一浩典, 宮下正弘, 宮川 恒, 森田勇人  
第 56 回 NMR 討論会, 首都大学東京, Nov. 14, 2017

**藍色細菌 *Anabaena variabilis* 由来 RNA 結合タンパク質 RbpD の構造機能相関**

田中邑樹, 佐藤直樹, 林 秀則, 森田勇人  
第 56 回 NMR 討論会, 首都大学東京, Nov. 14, 2017

**トリス (ピピリジル) 遷移金属 (II) 塩化物のトリス (オキサラト) アルミ (III) 酸のナトリウム塩とカリウム塩による反応性の違い**

原川和也, 宮前 博  
日本化学会第 96 春季年会 (京都) 2016 年 3 月, 講演要旨集, 3PA-004

**銅 (I) イソシアニド錯体の発光特性**

早川拓弥, 谷原佑輔, 橋本雅司, 寺前裕之, 宮前 博, 阪田知巳  
第 77 回応用物理学会秋季学術講演会 (新潟) 2016 年 9 月, 講演要旨集, 16p-P6-2

**OLED 用発光性 Cu (I) 錯体の開発**

阪田知巳, 早川拓弥, 谷原佑輔, 橋本雅司, 寺前裕之, 宮前 博  
第 33 回「センサ・マイクロマシンと応用システム」シンポジウム (平戸) 2016 年 10 月, 講演要旨集, 25am2-PS-019

**Synthesis of Copper (I) Complex with Cu-C Bond for Photoluminescent Devices**

Takuya Hayakawa, Yusuke Yabara, Masashi Hashimoto, Hiroyuki Teramae, Hiroshi Miyamae, Tomomi Sakata  
29th International Microprocesses and Nanotechnology Conference (Kyoto), November 2016, 11P-11-97

**銅 (I) イソシアニド錯体の発光過程の検討**

早川拓弥, 橋本雅司, 寺前裕之, 宮前 博, 阪田知巳  
第 64 回応用物理学会春季学術講演会 (横浜) 2017 年 3 月, 講演要旨集, 15a-P8-26

**メラミンを配位子とする発光性 Cu (I) 錯体の検討**

松田久睦, 谷原佑輔, 島田康弘, 早川拓弥, 阪田知巳  
第 64 回応用物理学会春季学術講演会 (横浜) 2017 年 3 月, 講演要旨集, 15a-P8-27

**銅 (I) イソシアニド錯体のソルバトクロミズム**

早川拓弥, 南山知花, 阪田知巳

第 78 回応用物理学会秋季学術講演会 (福岡) 2017 年 9 月, 講演要旨集, 5p-PA2-29

**有機溶媒検知センサを目指した銅 (I) 錯体のソルバトクロミズム現象**

早川拓弥, 南山知花, 阪田知巳

第 34 回「センサ・マイクロマシンと応用システム」シンポジウム (広島) 2017 年 10 月, 講演要旨集, 01am2-PS-163

**Substituent effects on the defunctionalization of alkylated single-walled carbon nanotubes**Yuya Takehana<sup>\*1</sup>, Mitsuaki Suzuki<sup>\*1,2</sup>, Michio Yamada<sup>\*1</sup>, Yutaka Maeda<sup>\*1</sup> (\*1 Department of Chemistry, Tokyo Gakugei University, \*2 Present Addresses: Department of Chemistry, Faculty of Science, Josai University)

The 50th Fullerene-Nanotube-Graphene General Symposium, Abstracts, 2P-12, p101, Tokyo, Japan, Feb. 21, 2016.

**Preparation, Structural Determination, and Characterization of Electronic Properties of Carbosilylated  $\text{Sc}_3\text{N}@I_h\text{-C}_{80}$** Takeshi Sugiura<sup>\*1</sup>, Shinpei Fukazawa<sup>\*1</sup>, Kyosuke Miyabe<sup>\*1</sup>, Masahiro Kako<sup>\*1</sup>, Masanori Yasui<sup>\*1</sup>, Michio Yamada<sup>\*2</sup>, Mitsuaki Suzuki<sup>\*2,5</sup>, Yutaka Maeda<sup>\*2</sup>, Takeshi Akasaka<sup>\*2,3,4</sup> (\*1 Department of Engineering Science, The University of Electro-Communications, \*2 Department of Chemistry, Tokyo Gakugei University, \*3 Life Science Center of Tsukuba Advanced Research Alliance, University of Tsukuba, \*4 Foundation for Advancement of International Science, \*5 Present Addresses: Department of Chemistry, Faculty of Science, Josai University)

The 50th Fullerene-Nanotube-Graphene General Symposium, Abstracts, 3P-4, p142, Tokyo, Japan, Feb. 22, 2016.

**単層カーボンナノチューブのアルキル化反応による発光特性の制御**前田 優<sup>\*1</sup>, 武埜祐哉<sup>\*1</sup>, 山田道夫<sup>\*1</sup>, 鈴木光明<sup>\*1,3</sup>, 村上達也<sup>\*2</sup> (\*1 東学芸大教, \*2 京大 iCeMS, \*3 現在の所属: 城西大理)

第 27 回基礎有機化学討論会要旨集, 39, 日本・広島, 9 月, 2016.

**Control of photoluminescence properties of single-walled carbon nanotubes**Yutaka Maeda<sup>\*1</sup>, Yuya Takehana<sup>\*1</sup>, Akane Nishino<sup>\*1</sup>, Shun Minami<sup>\*1</sup>, Michio Yamada<sup>\*1</sup>, Mitsuaki Suzuki<sup>\*1,3</sup>, Shigeru Nagase<sup>\*2</sup> (\*1 Department of Chemistry, Tokyo Gakugei University, \*2 Fukui Institute for Fundamental Chemistry, Kyoto University, \*3 Present Addresses: Department of Chemistry, Faculty of Science, Josai University)

The 51th Fullerene-Nanotube-Graphene General Symposium, Abstracts, 1-2, p10, Sapporo, Japan, 7. Sep. 2016.

**Utilizing a caged electron spin of an endohedral metallofullerenes for molecular location sensing**

Yuta Takano<sup>\*1</sup>, Ryo Tashita<sup>\*2</sup>, Mitsuaki Suzuki<sup>\*3,4</sup>, Shigeru Nagase<sup>\*5</sup>, Hiroshi Imahori<sup>\*1,6</sup>, Takeshi Akasaka<sup>\*2,3,7,8</sup> (\*1 Institute for Integrated Cell-Material Sciences (WPI-iCeMS) Kyoto University, \*2 Life Science Center of Tsukuba Advanced Research Alliance University of Tsukuba, \*3 Department of Chemistry, Tokyo Gakugei University, \*4 Department of Chemistry, Josai University, \*5 Fukui Institute for Fundamental Chemistry, Kyoto University, \*6 Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, \*7 Foundation for Advancement of International Science, \*8 State Key Laboratory of Materials Processing and Die & Mold Technology School of Materials Science and Engineering, Huazhong University of Science and Technology)

The 51th Fullerene-Nanotube-Graphene General Symposium, Abstracts, 2-4, p25, Sapporo, Japan, 8. Sep. 2016.

**Competitive elimination and decomposition reaction of oxidized single-walled carbon nanotubes depending on the degree of functionalization**

Yutaka Maeda<sup>\*1</sup>, Erika Sone<sup>\*1</sup>, Akane Nishino<sup>\*1</sup>, Yuri Amagai<sup>\*1</sup>, Wei-Wei Wang<sup>\*2</sup>, Michio Yamada<sup>\*1</sup>, Mitsuaki Suzuki<sup>\*1,6</sup>, Jun Matsui<sup>\*3</sup>, Masaya Mitsuishi<sup>\*4</sup>, Toshiya Okazaki<sup>\*5</sup>, Shigeru Nagase<sup>\*2</sup> (\*1 Department of Chemistry, Tokyo Gakugei University, \*2 Fukui Institute for Fundamental Chemistry, Kyoto University, \*3 Department of Material and Biological Chemistry, Yamagata University, \*4 Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, \*5 CNT-Application Research Center, National Institute of Advanced Industrial Science and Technology (AIST), \*6 Present Addresses: Department of Chemistry, Faculty of Science, Josai University)

The 52th Fullerene-Nanotube-Graphene General Symposium, Abstracts, 3-3, p34, Tokyo, Japan, 3. March. 2017.

**Molecular location recognizing approach by the anisotropic magnetic property of an endohedral metallofullerene Ce@C<sub>82</sub>**

Yuta Takano<sup>\*1</sup>, Ryo Tashita<sup>\*2</sup>, Mitsuaki Suzuki<sup>\*2,3</sup>, Shigeru Nagase<sup>\*4</sup>, Hiroshi Imahori<sup>\*1</sup>, Takeshi Akasaka<sup>\*2</sup> (\*1 Institute for Integrated Cell-Material Sciences (WPI-iCeMS), Kyoto University, \*2 Life Science Center of Tsukuba Advanced Research Alliance, University of Tsukuba, \*3 Department of Chemistry, Josai University, \*4 Fukui Institute for Fundamental Chemistry, Kyoto University)

The 97th Annual Meeting of The Chemical Society of Japan, Abstracts, 3F7-38, Yokohama, 16-19. March, 2017.

**Structural analysis of non-IPR endohedral metallofullerenes (Invited Speaker)**

Mitsuaki Suzuki<sup>\*1</sup>, Takeshi Akasaka<sup>\*2</sup> (\*1 Department of Chemistry, Josai University, \*2 Foundation for Advancement of International Science)

The 2nd International Symposium on NanoCarbon (ISNC2017), Wuhan, China, 23-27. June, 2017.

### **Effect of Initial Degree of Functionalization of Alkylated Single-Walled Carbon Nanotubes on Their Thermal Stability and Photoluminescence Properties**

Yutaka Maeda<sup>\*1</sup>, Yuya Takehana<sup>\*1</sup>, Jing-Shuang Dang<sup>\*2</sup>, Mitsuaki Suzuki<sup>\*1,3</sup>, Michio Yamada<sup>\*1</sup>, Shigeru Nagase<sup>\*2</sup> (\*1 Department of Chemistry, Tokyo Gakugei University, \*2 Fukui Institute for Fundamental Chemistry, Kyoto University, \*3 Present Addresses: Department of Chemistry, Faculty of Science, Josai University)

The 53th Fullerene-Nanotube-Graphene General Symposium, Abstracts, 3P-5, p123, Kyoto, Japan, Sep. 15, 2017.

### **ソルボサーマル法による金属ポルフィリン超分子の合成と構造決定**

安達裕紀, 鈴木光明, 秋田素子 (城西大理)

第 11 回有機 $\pi$ 電子系シンポジウム要旨集, PB23, 埼玉, 2017 年 12 月

### **ハト羽毛ケラチン calamus 遺伝子のクローニング**

高橋理恵子

第 89 回日本生化学会大会 (仙台), 2016 年 9 月, 講演要旨集, p. 305

### **Molecular cloning of scale keratin genes of pigeon**

高橋理恵子

第 90 回生命科学系学会合同年次大会 (神戸), 2017 年 12 月, 講演要旨集, p. 480

### **D. virilis 及び D. laticola におけるペプチドグリカン認識タンパク-LB (PGRP-LB) の発現調節**

北川浩子

第 89 回日本生化学会 (仙台), 2016 年 9 月, 3P-224

### **ギフチョウ属の食草選択に関わる遺伝子の同定**

北川浩子

生命科学系学会合同年次大会, 第 40 回日本分子生物学会, 第 90 回日本生化学会 合同大会 (神戸), 2017 年 12 月, 3P-713

### **埼玉県入間川水系および東京都多摩川水系を中心としたヌマエビ科の分布調査**

石黒直哉, 田村直輝, 大柏愛実

日本甲殻類学会第 54 回大会 (鹿児島), 2016 年 10 月

### **埼玉県入間川水系における在来種ヌマエビの生息域と外来カワリヌマエビ属の侵入状況**

石黒直哉, 田村直輝, 大柏愛実

DNA 鑑定学会第 9 回大会 (東京), 2016 年 11 月

### **淡水エビ分布状況調査を目的とした環境 DNA 分析手法の開発**

石黒直哉, 飯島大智, 石田季久

日本 DNA 多型学会第 25 回学術集会 (千葉), 2016 年 12 月

**福井県越前市域におけるドジョウ (*Misgurnus anguillicaudatus*) の遺伝的特性**日和佳政<sup>\*1</sup>, 高橋将人, 藤長裕平<sup>\*1</sup>, 石黒直哉 (\*1 越前市産業環境部)

日本 DNA 多型学会第 25 回学術集会 (千葉), 2016 年 12 月

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石黒直哉, 石田季久, 飯島大智

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**mtDNA CO II 遺伝子領域の解析によるゲンジボタルの養殖個体と野生個体の地域個体群の判定**齊藤達也, 加藤太郎<sup>\*1</sup>, 石黒直哉 (\*1 鹿大)

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2017 年光化学討論会, 東北大学青葉山キャンパス (宮城), 2017 年 9 月, 3B07

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日本化学会第 97 春季年会, 慶応大学日吉キャンパス (神奈川), 2017 年 3 月, 3B5-36

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宇和田貴之, 佐藤美波, 石川 満

2016 年光化学討論会, 東京大学駒場キャンパス (東京), 2016 年 9 月, 1P020

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UWADA, Takayuki; TAKENAKA, Yoshiki; YOSHIDA, Kazuki; ISHIKAWA, Mitsuru

日本化学会第 96 春季年会, 同志社大学京田辺キャンパス (京都), 2016 年 3 月, 2PA-067

**Formation of photoluminescent Au cluster encapsulated in protein assisted by UV light irradiation**

T. Uwada, Y. Takenaka, K. Yoshida, and M. Ishikawa

日本化学会第 96 春季年会 (京都), 2016 年 3 月

**Polymorphism of perylene nanocrystals in polymer matrices studied by single particle spectroscopy**

T. Uwada, M. Sato, M. Ishikawa

2016 年光化学討論会 (東京), 2016 年 9 月

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2016 年光化学討論会 (東京), 2016 年 9 月

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宇和田貴之, 佐藤美波, 石川 満

日本化学会第 97 春季年会 (神奈川), 2017 年 3 月

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2017 年光化学討論会 (仙台), 2017 年 9 月

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2017 年光化学討論会 (仙台), 2017 年 9 月

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宇和田貴之, 鈴木千加, 高橋郁也, 石川 満

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日本化学会第 6 回 CSJ 化学フェスタ 2016 (船堀), 2016 年 10 月, 講演要旨集, P9-034

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日本化学会第 97 回春季年会 (慶応大理工), 2017 年 3 月, 講演要旨集, 1PB-058

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2017 年光化学討論会 (仙台), 2017 年 9 月, 講演要旨集, 3P33

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日本化学会第 7 回 CSJ 化学フェスタ 2017 (船堀), 2017 年 10 月, 講演要旨集, P7-027

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CSJ フェスタ 2017 (船堀), 2017 年 10 月

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5th Ito international Research Center conference (IIRC5) (Tokyo), 2017 年 11 月

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