ISSN 0919-4614

SCIENCE BULLETIN OF JOSAI UNIVERSITY

城西大学理学部研究報告

Vol. 25 March 2021

FACULTY OF SCIENCE
JOSAI UNIVERSITY
SAKADO, SAITAMA, JAPAN

SCIENCE BULLETIN OF JOSAI UNIVERSITY

城西大学理学部研究報告

Vol. 25　March 2021

CONTENTS

PART I ANNUAL REPORTS

1. Abstracts of Papers Published in Journals

MATHEMATICS

Semilocal monodromy of rigid local systems

T. Oshima
Formal and Analytic Solutions of Diff. Equations, *Springer Proceedings in Mathematics and Statistics* **256** (2018), 189–199.

The rigid local system on $\mathbb{P}^1 \setminus S$ with a set S of finite points is realized as a rigid Fuchsian differential equation M of Schlesinger canonical form. Here "rigid" means that the equation is uniquely determined by the equivalence classes of residue matrices of M at the points in S. The semilocal monodromy in this paper is the conjugacy class of the monodromy matrix obtained by the analytic continuation of the solutions of M along an oriented simple closed curve γ on $\mathbb{C} \setminus S$. Since it corresponds to the sum of residue matrices at the singular points surrounded by γ and the equation M is obtained by applying additions and middle convolutions to the trivial equation, we study the application of the middle convolution to the sums of residue matrices. In this way we give an algorithm calculating this semilocal monodromy, which also gives the local monodromy at the irregular singular point obtained by the confluence of these points.

Confluence and versal unfolding of Pfaffian systems

T. Oshima
Josai Mathematical Monographs **12** (2020), 117–151.

A versal unfolding of a Pfaffian system with irregular singularities on the Riemann sphere is studied through its middle convolution. If the system is rigid, it is realized as a confluent limit of a rigid Fuchsian system. We show that the versal unfolding of a rigid Pfaffian system is extended to a versal KZ equation regarding singular points as variables. Appell's hypergeometric equations and their confluences are the simple examples.

A characterization of the monodromy group of Gauss hypergeometric equation.

T. Oshima and K. Shimizu
Josai Mathematical Monographs **12** (2020), 153–161.

We give a characterization of the monodromy group of the second order linear Fuchsian differential equation on the Riemann sphere which has three singular points.

Local functional equations attached to the polarizations of homaloidal polynomials.

Takeyoshi Kogiso1, and Fumihiro Sato[*1] (*1 Institute for Mathematics and Computer Science Tsuda College)
Kyushu J. Math. **72** (2018), no. 2, 307-331.

An identity that relates the Fourier transform of a complex power of homogeneous polynomial functions on a real vector space with a complex power of homogeneous polynomial functions on the dual vector space is called a local functional equation. A rich source of polynomials satisfying local functional equations is the theory of prehomogeneous vector spaces. Almost all known examples of local functional equations are of this type. However, recently, local functional equations of non-prehomogeneous type have been found. In this paper we present new examples of non-prehomogeneous polynomials satisfying a local functional equation. More precisely, we prove a local functional equation for the polarization of an arbitrary homaloidal polynomial, and calculate the associated b-function identities explicitly.

Kauffman bracket polynomials of Conway Coxeter friezes.,

Takeyoshi Kogiso, and Michihisa Wakui[*1] (*1 Department of Mathematics, Faculty of Engineering Science, Kansai University)
Proceedings of the Meeting for Study of Number Theory, *Hopf Algebras and Related Topics*, 51-79, Yokohama Publ., Yokohama, 2019.

In this paper, we construct Kauffman bracket polynomials associated with Conway Coxeter Friezes of zigzag type based on Yamada's ancestor triangles and we denote the relation between Conway Coxeter Friezes of zigzag type and Yamada's ancestor triangles. Furthermore we also explain relations between Conway Coxeter Friezes of zigzag type and Markov triples.

A bridge between Conway-Coxeter friezes and rational tangles through the Kauffman bracket polynomials.,

Takeyoshi Kogiso1, and Michihisa Wakui[*1] (*1 Department of Mathematics, Faculty of Engineering Science, Kansai University)
J. Knot Theory Ramifications **28** (2019), no. 14, 1950083, 40 pp.

In this paper, we build a bridge between Conway – Coxeter friezes (CCFs) and rational tangles through the Kauffman bracket polynomials. One can compute a Kauffman bracket polynomial attached to rational links by using CCFs. As an application, one can give a complete invariant on CCFs of zigzag-type.

Traveling wave solutions for a predator-prey system with two predators and one prey

J.-S. Guo[*1], K.-I. Nakamura[*2], T. Ogiwara, C.-C. Wu[*3] (*1Tamkang University, *2 Kanazawa University, *3 National Chung Hsing University)
Nonlinear Analysis: Real World Applications **54** (2020), 103111.

We study a predator-prey model with two alien predators and one aborigine prey in which the net growth rates of both predators are negative. We characterize the invading speed of these two predators by the minimal wave speed of traveling wave solutions connecting the predator-free state to the co-existence state. The proof of the existence of traveling waves is based on a standard method by constructing (generalized) upper-lower-solutions with the help of Schauder's fixed point theorem. However, in this three species model, we are able to construct some suitable pairs of upper-lower-solutions not only for the super-critical speeds but also for the critical speed. Moreover, a new form of shrinking rectangles is introduced to derive the right-hand tail limit of wave profile.

Convergence and structure theorems for order-preserving dynamical systems with mass conservation

T. Ogiwara, D. Hilhorst[*1], H. Matano[*2] (*1 CNRS, Université de Paris-Sud, *2 Meiji University)
Discrete and Continuous Dynamical Systems - A **40** (2020), 3883-3907.

We establish a general theory on the existence of fixed points and the convergence of orbits in order-preserving semi-dynamical systems having a certain mass conservation property (or, equivalently, a first integral). The base space is an ordered metric space and we do not assume differentiability of the system nor do we even require linear structure in the base space. Our first main result states that any orbit either converges to a fixed point or escapes to infinity (convergence theorem). This will be shown without assuming the existence of a fixed point. Our second main result states that the existence of one fixed point implies the existence of a continuum of fixed points that are totally ordered (structure theorem). This latter result, when applied to a linear problem for which 0 is always a fixed point, automatically implies the existence of positive fixed points. Our result extends the earlier related works by Arino (1991), Mierczyński (1987) and Banaji-Angeli (2010) considerably with exceedingly simpler proofs. We apply our results to a number of problems including molecular motor models with time-periodic or autonomous coefficients, certain classes of reaction-diffusion systems and delay-differential equations.

Asymptotic properties of solutions of a Lanchester-type model

T. Ito[*1], T. Ogiwara, H. Usami[*2] (*1 Nikko City Inokura Elementary School, *2 Gifu University)

Differential Equations and Applications **12** (2020), 1–12.

An ordinary differential system referred to as Lanchester-type model is studied. Asymptotic properties of solutions for such systems are considered. In particular, we examine how the limit of the solution as time tends to the infinity varies according to the initial data and we find asymptotic form of solutions that decay to (0,0).

The sign of traveling wave speed in bistable dynamics

J.-S. Guo[*1], K.-I. Nakamura[*2], T. Ogiwara, C.-H. Wu[*3] (*1 Tamkang University, *2 Kanazawa University, *3 National Chiao Tung University)
Discrete and Continuous Dynamical Systems - A **40** (2020), 3451–3466.

We are concerned with the sign of traveling wave speed in bistable dynamics. This question is related to which species wins the competition in multiple species competition models. It is well-known that the wave speed is unique for traveling wave connecting two stable states. In this paper, we first review some known results on the sign of wave speed in bistable two species competition models. Then we derive rigorously the sign of bistable wave speed for a special three species competition model describing the competition in two different circumstances: (1) two species are weak competitors and one species is a strong competitor; (2) three species are very strong competitors. It is interesting to observe that, under certain conditions on the parameters, two weaker competitors can wipe out the strongest competitor.

Stability and uniqueness of traveling waves for a discrete bistable 3-species competition system

J.-S. Guo[*1], K.-I. Nakamura[*2], T. Ogiwara, C.-C. Wu[*3] (*1 Tamkang University, *2 Kanazawa University, *3 National Chung Hsing University)
Journal of Mathematical Analysis and Applications **472** (2019), 1534–1550.

We study the stability and uniqueness of nonzero speed traveling waves for a threecomponent lattice dynamical system. This system arises in the study of three species competition model in which there is no competition between the first and the third species. Under the bistable consideration, we first derive the strict monotonicity of nonzero speed traveling waves. Then some super-sub-solutions are constructed based on these strictly monotone traveling waves. Finally, utilizing the constructed supersub-solutions, we prove the stability and uniqueness of nonzero speed traveling waves of this system.

On the behavior of solutions for Lanchester square-law models with timedependent coefficients

T. Ogiwara, H. Usami[*] (* Gifu University)

Josai Mathematical Monographs **11** (2018), 15–25.

This paper concerns an ordinary differential system which is a so-called Lanchester square-law model with time-dependent coefficients. We study qualitative properties of solutions and, among other things, discuss the relation between behavior of solutions and their initial data.

On quaternioic 3 CR-structure and pseudo-Riemannian metric

Y. Kamishima
Applied Math. **9** (2) 114–129 (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*, which is a generalization of *QCR*-structure on a $4n+3$-manifold M.

Homogeneous Sasaki and Vaisman manifolds of unimodular Lie groups

D. Alekseevsky, K. Hasegawa, Y. Kamishima
Nagoya Math. Jour. (https://doi.org/10.1017/nmj. 2019.34.)

We show a basic structure theorem of simply connected homogeneous Sasaki and Vaisman manifods of unimodular Lie groups, up to holomorphic isometry.

Locally homogeneous aspherical Sasaki manifolds

O. Baues, Y. Kamishima
Differential Geom. Appl. **70** (2020), 101607, 41 pp.

We proved that any compact regular aspherical Sasaki manifold with solvable fundamental group is nitely covered by a Heisenberg manifold and its Sasaki structure may be deformed to a locally homogeneous one.

On the Stokes geometry of a unified family of (P_J)-hierarchies (J=I, II, IV, 34)

Yoko Umeta
Publications of the Research Institute for Mathematical Sciences **55**, (2019) 79–107.

In this paper, the Stokes geometry for a unified family of (P_J)-hierarchies (J=I, II, IV, 34) with a large parameter is studied. For the unified family of (P_J)-hierarchies, we give the underlying Lax pair and study the relation between the Stokes geometry of the system of nonlinear ordinary differential equations and that of its underlying Lax pair by using the

explicit forms of 0-parameter solutions.

General formal solutions for a unified family of (P_J)-hierarchies (J=I, II, IV, 34)

Yoko Umeta
Journal of the Mathematical Society of Japan **71**, No.3, (2019) 979-1003.

A unified family of (P_J)-hierarchies (J=I, II, IV, 34) with a large parameter is introduced. The family has many parameters and we can obtain each of the (P_J)-hierarchies by taking special values of the parameters. In this paper, general formal solutions which are called instanton-type solutions for the system are constructed.

A certain property of a unified family of (P_J)-hierarchies (J=I, II, IV, 34) with a large parameter

Yoko Umeta
RIMS Kôkyûroku Bessatsu **B75** (2019), 101-111.

In this paper, the deformation equation and the Schrödinger equation associated with a unified family of (P_J)-hierarchies are derived from the underlying Lax pair.

Uniqueness of polarization for the autonomous 4-dimensional Painlevé-type systems

A. Nakamura, E. Rains
International Mathematical Research Notices (2020), https://doi.org/10.1093/imrn/rnaa037.

We prove that for any autonomous 4-dimensional integral system of Painlevé type, the Jacobian of the generic spectral curve has a unique polarization, and thus by Torelli's theorem cannot be isomorphic as an unpolarized abelian surface to any other Jacobian. This enables us to identify the spectral curve and any irreducible genus 2 component of the boundary of an affine patch of the Liouville torus.

The Painlevé divisors of the autonomous 4-dimensional Painlevétype equations

A. Nakamura
RIMS Kôkyûroku Bessatsu, **B78**, pp.29-50, 2020.

Following 'Algebraic integrability, Painlevé geometry and Lie algebras' by Adler, van Moerbeke, and Vanhaecke, we consider compactification of the Liouville tori for the autonomous 4- dimensional Painlevétype equations by adjoining the Painlevé divisors. We can see that the genus 2 components of the Painlevé divisors are all isomorphic to the corresponding spectral curve. We illustrate the motivating examples for 'Uniqueness of polarization for the autono-

mous 4-dimensional Painlevétype systems', which asserts that the genus 2 curves are uniquely determined by the Liouville tori of the autonomous 4-dimensional Painlevétype equations. This may enable us to recover a linear problem from the nonlinear integrable systems.

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

A. Nakamura
Annales de l'Institut Fourier, **vol. 69, no. 2**, pp. 845–893, 2019.

In recent studies, 4-dimensional analogs of the Painlevé equations were listed and there are 40 types. The aim of the present paper is to geometrically characterize these 40 Painlevé-type equations. For this purpose, we study the autonomous limit of these equations and degeneration of their spectral curves. The spectral curves are 2-parameter families of genus two curves and their generic degeneration are one of the types classified by Namikawa and Ueno. Liu's algorithm enables us to find the degeneration types of the spectral curves for our 40 types of integrable systems. This result is analogous to the following fact; the families of the spectral curves of the autonomous 2-dimensional Painlevé equations P_{I}, P_{II}, P_{IV}, P_{III}^{D8}, P_{III}^{D7}, P_{III}^{D6}, P_{V} and P_{VI} define elliptic surfaces with the singular fiber at $H = \infty$ of the Dynkin types $E_8^{(1)}$, $E_7^{(1)}$, $E_6^{(1)}$, $D_8^{(1)}$, $D_7^{(1)}$, $D_6^{(1)}$, $D_5^{(1)}$ and $D_4^{(1)}$, respectively.

Degeneration scheme of 4-dimensional Painlevé-type equations

H. Kawakami, A. Nakamura, H. Sakai
MSJ Memoir, **vol. 37**, pp.25–111, 2018.

There are four 4-dimensional Painlevé-type equations derived from isomonodromic deformation of the Fuchsian equations: they are the Garnier system in two variables, the Fuji-Suzuki system, the Sasano system, and the sixth matrix Painlevé system. We degenerate these four source equations, and systematically obtain other 4-dimensional Painlevé-type equations, whose associated linear equations are of unramified type. There are 22 types of 4-dimensional Painlevé-type equations: 9 of them are partial differential equations, 13 of them are ordinary differential equations. Some well-known equations such as the Noumi-Yamada systems are included in this list. They are expressed as Hamiltonian systems, and their Hamiltonians are simply written by using the Hamiltonians of the classical Painlevé equations.

Simulation of leukopenia developed with influenza A/H5N1 and its recovery with treatment of antibody to influenza A/H5N1 virus

H.Yasuda, S.Kawachi, K.Suzuki
ADC Letter for Infectious Disease Control, **7** (1), (2020) 29–33.

White blood cell count rapidly decreases after onset and engender leukopenia in case of highly pathogenic avian influenza A/H5N1. Numerical simulations were conducted using a mathematical model of mice to elucidate the pathogenesis of leukopenia.

COVID-19 in the 23 wards of Tokyo from April 6th to June 14th, 2020

F. Ito, H.Yasuda, K. Suzuki
ADC Letter for Infectious Disease Control, **7** (2), (2020) 72–75.

We focused on the epidemic of COVID-19 in Tokyo's 23 wards in Tokyo metropolitan area from April 6th to June 14th. The 23 wards are separated clearly three zones such as Zone 1, 2 and 3 by the epidemic of COVID-19: Zone 1 downtown, Zone 2 inside of JR-Yamanote Line, and Zone 3 residential areas.

Sum types of uncertainty relations for generalized quasi-metric adjusted skew informations

Kenjiro Yanagi
International Journal of Mathematical Analysis and Applications, **vol.5,** no.4, 2018, pp.85–94

It is well known that almost all uncertainty relations including Heisenberg uncertainty relation and Schrodinger uncertainty relation were given by product types of trace inequalities. This is why these results were proved by Schwarz's inequality. These product types of uncertainty relations were extended to the case of not necessarily hermitian quantum mechanical observables and positive operators representing quantum states. On the other hand, sum types of uncertainty relations were given for arbitrary finite N not necessarily hermitian quantum mechanical observables. Some uncertainty relations are presented by generalized quasi-metric adjusted skew informations for two different generalized states. These uncertainty relations are nontrivial as long as the observables are mutually noncommutative. The relations among these new and existing uncertainty inequalities have been investigated. Finally, the reverse inequalities of the sum types of uncertainty relations are obtained.

On the trace inequalities related to left-right multiplication operators and their applications

Kenjiro Yanagi
Linear and Nonlinear Analysis, **vol.4,** no.3, 2018, pp.361–370

Recently we obtained non-hermitian extensions of Heisenberg type and Schrodinger type uncertainty relations for generalized quasi-metric adjusted skew information or generalized quasimetric adjusted correlation measure and applied to the inequalities related to fidelity and trace distance for different two generalized states which were given by Audenaert et al; and

Powers-Stormer. In this paper we state the properties of left or right multiplication operators and obtain some related inequalities.

Noncommutative versions of inequalities in quantum information Theory

Ali Dadkhan[*1], Mohammad Sal Moslehian[*1], Kenjiro Yanagi (*1 Department of Pure Mathematics Ferdowsi University of Mashhad)
Analysis and Mathematical Physics, **vol.9,** no.4, 2019, pp.2151–2169

In this paper, we aim to replace in the definitions of covariance and correlation the usual trace Tr by a tracial positive map between unital C*-algebras and to replace the functions x^α and x^{1−α} by two functions f and g satisfying some mild conditions. These allow us to define the generalized covariance, the generalized variance, the generalized correlation and the generalized Wigner-Yanase-Dyson skew information related to the tracial positive maps and functions f and g. We present a generalization of Heisenberg's uncertainty relation in the noncommutative framework. We extend some inequalities and properties for the generalized correlation and the generalized Wigner-Yanase-Dyson skew information. Furthermore, we extend some inequalities for the generalized skew information such as uncertainty relation and the relation between the generalized variance and the generalized skew information.

Refined Hermite-Hadamard inequality and weighted logarithmic mean

Kenjiro Yanagi
Linear and Nonlinear Analysis, **vol.6, no.2**, 2020, pp.167–177

Inspired by the recent works by R.Pal et al., and Furuichi-Minculete, we give further refined inequalities for a convex Riemann integrable function, applying the refined Hermite Hadamard inequality. Our approach is different from their one in their papers. As corollaries, we give the refined two types of inequalities on the weighted logarithmic mean. At last we give corresponding operator inequalities.

Asymptotic behavior of regularized estimator under multiple and mixed-rates asymptotics

Shimizu, Y.
Josai Mathematical Monographs, **11** (1), pp.3–14, 2018.

In this paper, we generalize the form of regularization terms considered in Masuda and Shimizu (2017), and derive the asymptotic behaviors including the moment convergence of estimators. Our setting includes sparsely regularized M-estimation such that sparse-bridge, the smoothly clipped absolute deviation and Seamless-L0 regularization.

AIC for the non-concave penalized likelihood method

Umezu, Y.[*1] Shimizu, Y. Masuda, H.[*2] Ninomiya, Y.[*3] (*1 Nagasaki University, *2 Kyusyu University, *3 The Institute of Statistical Mthematics)
Annals of the Institute of Statistical Mathematics, **71** (2), pp.247-274, 2019.

In this paper, we derive an information criterion based on the original definition of the AIC by considering minimization of the prediction error rather than model selection consistency. Concretely speaking, we derive a function of the score statistic that is asymptotically equivalent to the non-concave penalized maximum likelihood estimator and then provide an estimator of the Kullback-Leibler divergence between the true distribution and the estimated distribution based on the function, whose bias converges in mean to zero.

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データサイエンスのための統計教育とその効果―統計解析ソフトウェア R を用いた授業の報告―

清水優祐
城西情報科学研究，**26** (1)，pp.17-22，2019

統計解析ソフトウェア R を用いたデータサイエンス教育のための授業内容と，その教育効果について報告した。

Python によるコード実装について―公開講座と数学セミナーの報告―

清水優祐
城西情報科学研究，**27** (1)，pp.8-43，2020

城西大学理学部数学科が主催している，高校生向け応用数学体験講座の内容と，数学科の学生が行ったアクティブラーニングの内容について，実際に作成した Python コードを紹介した。

CHEMISTRY

Ab initio electronic structure calculation of polymononucleotide, a model of B-type DNA

Hiroyuki Teramae, Yuriko Aoki
AIP Conference Proceedings **2040**, 020013 (2018); https://doi.org/10.1063/1.5079055

As an attempt at the electronic structure calculations of the B-type model-DNA, (poly-(guanine) poly-(cytosine)) double helix including sodium atoms as counter cations, 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. At the level of 6-31G basis sets, energy band structures were calculated for the polymers with and without sugar and sodium phosphate and found that the difference is very large when excluding the sodium phosphate. We also calculated the four single helix polymers in order to compare these band structures with the double helix polymononucleotide. The difference is not small especially for the guanine-cytosine polymer.

DNA の電子状態計算

寺前裕之，青木百合子[*1]（*1 九大）
J. Comp. Chem. Jpn, **16**, 157-159 (2017)（日本コンピューター化学会秋季年会 2017 年精選論文特集選出，出版は 2018 年）

As an electronic structure calculation of the B-type model-DNA, the calculation of (poly-(guanine) poly-(cytosine)) model polymer is performed by means of the ab initio crystal orbital method adapting the screw axissymmetry which results in great reduction of computational efforts. All sugar backbones and sodium phosphate are included in the calculations. Energy band structures are calculated at the 6-31G level. For a comparison, the calculation without sodium phosphate is also performed. The resultant energy band structure is very different from that of the original one and it should be concluded that the alkali phosphate is necessary to describe the electronic structure of model-DNA.

フェルラ酸のフリーラジカル消去能に関する理論的研究

寺前裕之，玄　美燕[*1]，山下　司[*1]，高山　淳[*1]，岡崎真理[*1]，坂本武史[*1]（*1 城西大薬）
J. Comp. Chem. Jpn, **17**, 150-152 (2018)（日本コンピューター化学会春季年会 2018 年精選論文特集選出）

Ferulic acid is known to have strong antioxidant properties. In the present study, we have investigated the electronic structures of Ferulic acid and its radical extracting the hydrogen atom from its phenolic hydroxyl group. We have discussed the relation of the results with the radical scavenging activity using the DPPH reagent measured by Xuan et al. We have found that the total energies of Ferulic acid derivatives and its radical species made from removing the hydrogen radical from the phenolic hydroxy group have the relation with the IC50 values. The orbital energies of the radical species also have the relation with the IC50 values. The deep learning study with the random forest model suggests that the contribution from α-SOMO and α-LUMO energies is important.

Practical Training in Simple Huckel Theory: Matrix Diagonalization for Highly Symmetric Molecules and Visualization of Molecular Orbitals

Shin-ichi Nagaoka[*1], Tatsunobu Kokubo[*2], Hiroyuki Teramae, Umpei Nagashima[*3] (*1 Ehime University, *2 Research Organization for Information Science and Technology, *3 FOCUS)

J. Chem. Educ., **95**, 1579–1586 (2018)

At an advanced stage of learning quantum chemistry, undergraduate students usually encounter simple Huckel-molecular orbital (HMO) theory, whose primitive approach gives very useful insight into the electronic structure of π-conjugated molecules. However, on one hand, computational HMO software, when programmed without using molecular symmetry, does not necessarily output chemically reasonable shapes of degenerate molecular-orbitals in benzene. On the other hand, separately inputting the molecular symmetry into the HMO calculation is mathematically redundant (i.e., duplicate information input). To solve this problem, in this study, a Microsoft Excel macro for obtaining reasonable HMOs of highly symmetric molecules such as benzene was developed. Furthermore, two other Excel macros for readily drawing quantitative contour plots of HMOs were created as studentfriendly tools. The practical training in simple HMO theory proposed in the present report using these three macros will be very useful for undergraduate teaching of quantum chemistry in terms of clearly showing the theoretical concept.

超高速クラスタ型並列計算機（京）を用いた汎用分子動力学プログラム LAMMPS の高速化

小久保達信[*1]，長岡伸一[*2]，寺前裕之，長嶋雲兵[*3]（*1 高度情報科学技術研究機構，*2 愛媛大，*3 FOCUS）
J. Comp. Chem. Jpn, **18** (4), 169–175 (2019); https://doi.org/10.2477/jccj.2019-0008.

分子動力学プログラム LAMMPS は，分散並列処理により高い効率で実装されており，スーパーコンピュータ「京」でも，大規模なノードを使ってもよくスケールし，高性能を発揮している．LAMMPS の さらなる高速化を目指し，Mod -FixLan 機能で利用されている乱数ルーチンの Single Instruction Multi Data（SIMD/ ベクトル）化及び OpenMP でのスレッド並列化によるさらなる高速化の実現を試みた．乱数生成は逐次処理のアルゴリズムが基本であり SIMD 化及び OpenMP による並列化の難しい部分の高速化を新たに実装した．特に乱数ルーチンの実装の改良によって，全体で 46% 程度の性能向上が観測された．まだまだ，LAMMPS には高速化の余地がある．

分子軌道計算と機械学習によるフェルラ酸の抗酸化作用の研究

寺前裕之，玄　美燕[*1]，山下　司[*1]，高山　淳[*1]，岡﨑真理[*1]，坂本武史[*1]（*1 城西大薬）
J. Comp. Chem. Jpn, **18** (5), 211–213 (2019); https://doi.org/10.2477/jccj.2019-0034
（日本コンピュータ化学会秋季年会 2019 年精選論文特集選出）

Ferulic acid is known to have strong antioxidant properties. In the present study, we investigate the electronic structures of ferulic acid and its radical species extracting the hydrogen atom from its phenolic hydroxyl group. The relation of the results by several machine learning models using R/caret package, such as partial least squares, random forest, radial basis function kernel regularized least squares, and baysian regularized neural network, with

the radical scavenging activity with the DPPH reagent, IC_{50}, measured by Sakamoto et al. is discussed. We found all four methods gave reasonable correlation coefficients which means the possible prediction of the IC_{50} values with the results of the molecular orbital calculations only.

Correlations of computational ionization energy with experimental oxidation potential and with antioxidant efficiencies in catechins

Shin-ichi Nagaoka[*1], Naofumi Nakayama[*2], Hiroyuki Teramae, Umpei Nagashima[*3] (*1 Ehime University, *2 CONFLEX Corporation, *3 FOCUS)
Chem. Phys., **522**, 77-83 (2019); https://doi.org/10.1016/j.chemphys.2019.02.002

Ionization energies of catechins were calculated by using B3LYP density functional method with 6-31G** basis set. Then, conformations of catechins were extensively explored. Geometry optimizations starting from the explored conformers were made not only for the neutral species but also for the radical cation. The ionization energy of each catechin was estimated as the energy difference between the most stable geometries obtained for the neutral species and radical cation. Tendency of experimental oxidation potential in catechins is well re-produced by this calculation, and the ionization energy correlates well with the singlet-oxygen quenching efficiency in case that stereochemistry of attachment at the 3-position is common. Electron transfer from catechins plays an important role in the singlet-oxygen quenching, free-radical scavenging and recycling from vitamin E radical to vitamin E. The reason for discrepancy among antioxidant efficiencies with regard to the ionization energy dependence is explained.

Possible Prediction of Molecular Properties with Machine Learning and Molecular Orbital Energies

Hiroyuki Teramae, Xuan Meiyan, Tsukasa Yamashita, Jun Takayama, Mari Okazaki, Takeshi Sakamoto
Proceedings of International Symposium on Environmental-Life Science and Nanoscales Technology 2019 (*ISENT2019*) pp.XVII-XXI (University of Yangon), September 2020.

The ferulic acid is known to have strong antioxidant properties. In the present study, we have investigated the electronic structures of the ferulic acid and its radical extracting the hydrogen atom from its phenolic hydroxyl group. We have discussed the relation of the results with the radical scavenging activity with the DPPH reagent, IC_{50}, measured by Sakamoto et al. by several machine learning models.

We use Gaussian16 program package to calculate the optimized geometries and the molecular orbitals of FA and its derivatives at RHF/6-31G** level and the radicals of FA and its derivatives which are made by removing the hydrogen atom from the phenolic hydroxyl group. The machine learning is performed with the R/caret packages.

We use the orbital energy levels of the radical forms of aSOMO, aSOMO-1, bSOMO, α

LUMO, and βLUMO, the neutral forms of HOMO-1, HOMO, LUMO, and LUMO+1, and the energy difference between the radical and neutral forms as the explanatory variables. We make the machine learning with these ten explanatory variables and IC_{50} value as the explained variable. For the regression method, we use partial least square, random forest, neural network, and krlsRadial.

All the methods give moderate/strong correlation coefficients and there should be a strong correlation. Furthermore, when we examine the machine learning with only the orbital energy levels of the radical forms, the correlation coefficients are almost the same.

In conclusion, we confirm the IC_{50} values of the ferulic acid can be predicted by just molecular orbital energies.

Addition to "Practical Training in Simple Hückel Theory: Matrix Diagonalization via Tridiagonalization, Cyclobutadiene, and Visualization of Molecular Orbitals"

Shin-ichi Nagaoka[*1], Yoshinori Yamasaki[*1], Hiroyuki Teramae, Umpei Nagashima[*2], and Tatsunobu Kokubo[*3] (*1 Ehime Universiy, *2 FOCUS *3 Research Organization for Information Science and Technology)

J. Chem. Educ. 2020, 97, 8, 2373-2374, https://doi.org/10.1021/acs.jchemed.0c00857

This paper is an addition to the article "Practical Training in Simple Hückel Theory: Matrix Diagonalization for Highly Symmetric Molecules and Visualization of Molecular Orbitals" by Shin-ichi Nagaoka, Tatsunobu Kokubo, Hiroyuki Teramae, and Umpei Nagashima. (1) Yoshinori Yamasaki, from the Department of Mathematics, Faculty of Science and Graduate School of Science and Engineering, Ehime University, Matsuyama 790-8577, Japan, is an author of this addition, together with the authors of the original article. With the addition, the new title of this work is "Practical Training in Simple Hückel Theory: Matrix Diagonalization via Tridiagonalization, Cyclobutadiene, and Visualization of Molecular Orbitals".

Synthesis and Evaluation of FICA Derivatives as Chiral Derivatizing Agents

Tomoyo Kamei[*1], Tamiko Takahashi[*1], Hiroyuki Teramae, Jyunichi Koyanagi[*1], (*1 Josai International University)

Chem. Pharm. Bull. **68**, 818-821 (2020)

1-Fluoroindan-1-carboxyic acid (FICA) derivatives containing a monosubstituted benzene ring (1b-e) were synthesized as their methyl esters and their potential as chiral derivatizing agents (CDAs) were assessed by both ^{19}F- and ^{1}H-NMR spectroscopy. Introduction of a substituent at the 4-position in the benzene ring caused a 1.2-2 fold increase in $\Delta\delta_F$ values when compared with that of FICA. This increase was investigated using a correlation model for ^{19}F-NMR and by the order of the stability of the *synperiplanar* (*sp*) and *antiperiplanar* (*ap*) conformers of the (*R,S*) and (*S,S*) diastereomers from the Gibbs' free energy at 298.15 K.

Three-Body Effects on the CO_2 Vibrational Frequency in van der Waals Trimers CO_2-M_2 (M=Kr, Xe, N_2) Investigated by Infrared Diode Laser Spectroscopy

Yasushi Ozaki

Proceedings of ICRINT2018, 433-436 (2019) (ISSN 2520-0186)

The vibrational frequency of CO_2 in the CO_2-containing van der Waals complex shifts from that of free CO_2 molecule due to the intermolecular interactions in the complex. When the CO_2-M moiety in the trimer has the same structure as the dimer, the relation $Dn_t = 2Dn_d$ is expected between the shifts in CO_2-M_2 trimer, Dn_t, and CO_2-M dimer, Dn_d, in the pairwise additive approximation. However, it is reported by Sperhac et al. (1996) that the $Dn_t/2Dn_d$ value for CO_2-Ar_2 and CO_2-Ar is 0.955, which is smaller than unity due to the three-body effect, although the CO_2-Ar in CO_2-Ar_2 trimer has the same T-shaped structure as CO_2-Ar dimer. In the present study, infrared spectra of CO_2-M and CO_2-M_2 (M=Kr, Xe) are measured by use of pulsed jet-diode laser apparatus in the CO_2 anti-symmetric vibration range. The anti-symmetric vibrational frequencies of CO_2 in CO_2-M_2 trimers are derived from the positions of strong Q-branch stacks in the spectra of CO_2-M_2. With the reported shifts in the dimers, the $Dn_t/2Dn_d$ values are calculated to be 0.956 for CO_2-Kr_2 and 0.954 for CO_2-Xe_2, which is in good agreement with CO_2-Ar_2, indicating that the three-body effects in these CO_2-rare gas complexes are the same. On the other hand, the $Dn_t/2Dn_d$ value for CO_2-$(N_2)_2$, is calculated to be 0.919 from the spectrum reported in Konno et al. (2011); the three-body effect in CO_2-$(N_2)_2$ is larger than those in CO_2-rare gas complexes.

Analyses of parameters affecting the fill factors of dye sensitized solar cells

Koichiro Mitsuke, Ryohei Watai, Katsunari Takuma, Takumu Fujiya

Proceedings of International Symposium on Environmental-Life Science and Nanoscales Technology 2019 (*ISENT2019*), the first of invited papers, 5 pages.

Dye-sensitized solar cells (DSSCs) consisting of multilayered nanocrystalline TiO_2 films, together with Ru complex dye N719, have been studied for the purpose of achieving economical photovoltaics with higher power conversion efficiencies and better durability. The efficiency of the DSSC is evaluated from the short-circuit current density J_{SC}, open circuit voltage V_{OC}, and fill factor *FF*. These parameters can be determined by measuring the current-voltage (J-V) curve under the illumination condition. The best fitting of the J-V data to the theoretical equation for an equivalent electric circuit

$$J_{SC} - J - \frac{V + JR_S}{R_{Sh}} - A\left\{\exp\left[\frac{F}{nRT}(V + JR_S)\right] - 1\right\} = 0 \qquad (1)$$

allowed the authors to evaluate the reverse saturation current density A of the diode, the shunt resistor R_{Sh}, and the series resistor R_S. Here, R_S includes the resistance due to FTO

glass substrate, that due to the redox reactions on Pt nanoparticles, and that due to diffusion of the carriers in the electrolyte. The optimized R_S values were in good agreement with those derived from electrochemical impedance spectroscopy (EIS). Influence of A and R_s on FF was discussed in terms of the absolute slope of the J-V curve in the vicinity of V_{OC}. The small-signal resistance was determined in two ways: either from the diameter of the largest semicircle in the Nyquist plots or from an analytical expression contributing to the above slope. The present results are the manifestation of the validity of the equivalent circuit employed and the individual resistances obtained by EIS.

Formulation of Raman scattering revisited.

R. Morita[*1], H. Morita, and M. Tasumi[*2] (*1 Josai Interrnational University, *2 University of Tokyo)
J. Raman Spect., **50**, (2019) 1245–1249.

In Raman scattering, photons are scattered by electrons in a molecule. Its mechanism was elucidated early after the development of quantum mechanics. If the frequencies of incident and scattered photons are denoted, respectively, by ν_0 and ν_s, the differential scattering cross section of a Raman band is proportional to $\nu_0\nu_s^3$. The differential scattering cross section of Rayleigh scattering is proportional to ν_s^4, as is known as the ν^4 rule. This article reconfirms these points from a tutorial viewpoint.

Heavy-metal stress response in cyanobacterium, *Synechococcus elongatus* PCC 7942.

E.H. Morita, S.M. Rahul[*1,2] and H. Hayashi[*2] (*1 Gyeongsang University, *2 Ehime University)
Proceedings of International Conference on Recent Innovations in Nanoscience & Technology 2018, (2019) 124–128.

For all living organisms, many of heavy metals are indispensable for specific physiological functions. Among these metals, Zn is the one being indispensable for proteins with zinc finger motifs. In spite of this strong necessity, presence of the excess amount of Zn^{2+} in cytosol is quite toxic for the cell. For a cyanobacterium, *Synechococcus elongatus* sp. PCC 7942, two proteins, SmtA and SmtB, those are coded in *smt* locus and transcribed divergently, regulate the cytosolic Zn^{2+} concentration properly. SmtA is the class-II metallothionein (56 aa), and SmtB is the repressor of *smtA* transcription (122 aa). Following Zn^{2+} binding with SmtB, DNA binding affinity of SmtB to the operator/promoter sequence of *smtA* goes down, and the transcription of *smtA* is induced.

To elucidate this molecular mechanism precisely, we prepared the series of point mutated or partially truncated SmtB, considering the chemical shift changes in heteronuclear multidimensional NMR spectra for ^{15}N and ^{13}C labelled SmtB following Zn^{2+} binding. For these mutated SmtB, we also analysed the inhibitory effect of Zn^{2+} binding, on the recognition of operator/promoter sequence of *smtA*, with EMSA technique. From these results, we have

succeeded to elucidate the molecular mechanism in which the structural change of SmtB following Zn^{2+} binding induces the loss the DNA binding affinity of SmtB to the operator/promoter sequence of *smtA*. This molecular mechanism is crucial for the heavy-metal stress response in cyanobacteria.

Secondary structural analysis of the cyanobacterial RNA-binding protein RbpD from cyanobacterium *Anabaena variabilis* with heteronuclear multi-dimensional NMR spectroscopy.

Y. Tanaka, N. Sato[*1], T. Sugiki[*2], H. Hayashi[*3] and E.H. Morita (*1 University of Tokyo, *2 Osaka University, *3 Ehime University)

Proceedings of International Conference on Recent Innovations in Nanoscience & Technology 2018, (2019) 148-152.

RbpD in *Anabena variabilis* is a member of the small RNA-binding proteins those contain a single RNA recognition motif (RRM). RNA-binding proteins are involved in proper control of gene expression, development and stress response, and is regarded as important factors in various organisms. In *A. variabilis,* low temperature induces the expression of *rbp* genes with the exception of *rbpD*. On the structural point of view, for *A. variabilis*, Rbps other than RbpD consist of an N-terminal RRM and a C-terminal glycine-rich domain, and RbpD only contains one RRM domain. To elucidate the functional differences of RRMs between RbpD and other Rbp proteins, especially RbpA1, we tried to compare the solution structure of RbpD with that of RbpA1, by heteronuclear multidimensional NMR spectroscopy. For this purpose, we have cloned the genes encoding RbpD and RbpA1, and introduced into an *E. coli* overexpression vector, pET-21a. Constructed plasmids were transferred into Rosetta Gami^{TM} B (DE3) / pLysS. Transferred *E. coli* was inoculated in M9 medium with the addition of ^{15}N-NH_4Cl and/or ^{13}C-Glucose at 37 °C. Overexpression of RbpD and RbpA1 were induced with the addition of 0.25 mM IPTG at OD_{600}=0.5, and further inoculated 3hours. Overexpressed proteins were purified with anion exchange and size exclusion chromatography. Purified proteins were concentrated to 0.25 mM. With these protein samples, we have measured the heteronuclear multidimensional NMR spectra with 700MHz FT-NMR (Varian; Josai Univ.), and 800MHz (Bruker; Osaka Univ). We have sequentially assigned the signals observed in these spectra and analyzed the secondary structures for RbpA1 and Rbp.

Solution structural studies of insecticidal peptide LaIT2 from Japanese scorpion, *Liocheles australasiae*, with heteronuclear multidimensional NMR spectroscopy.

M. Tamura, H. Juichi[*1], M. Miyashita[*1], H. Miyagawa[*1] and E. H. Morita (*1 Kyoto University)

Proceedings of International Conference on Recent Innovations in Nanoscience & Technology 2018, (2019) 129-133.

There are two scorpions in Japan. One inhabits in subtropical islands and the other, *Liocheles australasiae*, mainly inhabits in the Yaeyama island. *L. australasiae* has the series

Fig, 1 Amino acid sequence of LaIT2 and LaIT1

of peptide like poison, those specifically acting for insects. Among these poisons, we have focused our attention on LaIT2, (59AA), which not only be insecticidal, but also has antibacterial activities. For smaller poison, LaIT1, solution structure was already solved with heteronuclear multidimensional NMR spectroscopy (Horita *et al.*, 2011). LaIT1 only shows the insecticidal activity and has the homologous amino acid sequence with C-terminal region of LaIT2 (Fig. 1).

In this study, we aim to find out the relationships between two biochemical characters of LaIT2 (insecticidal and antibacterial activities) and structural factors derived those. For this purpose, we at first tried to construct the overexpression system for biochemically active LaIT2. The cDNA for LaIT2, optimized for the *E. coli* overexpression system was chemically synthesized, and introduced in the three overexpression vectors for *E. coli*, pET-21d, pET-32a, pCold^{TM}ProS2. Constructed plasmids were transferred to Rosetta-Gami^{TM} B (DE3)/pLysS, or BL21 (DE3)/pLysS. With these systems, isolated and purified LaIT2 was precipitated. In consideration of these results, we tried to solubilize the precipitated non-tagged proteins with 6M guanidine hydrochloride, and all cysteine residues were modified with TAPS-sulfonate. With these chemically modified peptides, we have optimized the refolding condition and we will show the results.

Heavy-metal sewage treatment system with cyanobacteria.

E.H. Morita and H. Hayashi

Proceedings of Internationa Conference on Recent Innovations in Nanoscience & Technology 2019 (2020) 12-15.

For all living organisms, many of heavy-metal ions are indispensable for the expression of specific physiological functions in proteins and so on. Within these heavy-meal ions, Zn^{2+} is specifically used in zinc finger proteins those specifically function at the molecular interaction surfaces such as those between protein and protein/DNA. In spite of this physiological importance, presence of the excess amount of Zn^{2+} in cytosol is quite toxic. In case for a cyanobacterium, *Synechococcus elongatus* PCC7942, two proteins, SmtA and SmtB, those are coded in *smt* locus and transcribed divergently, regulate the cytosolic Zn^{2+} concentration. SmtA is the class-II metallothionein (56 aa), and SmtB is the repressor of *smtA* transcription. Comparison of amino acid sequences between SmtA and mammalian metallothionein showed that the number of Zn^{2+} bound with SmtA is almost the half of that for mammalian metallothionein.
To certify this speculation and to clear the coordination style of Zn^{2+} in SmtA, we have constructed *E. coli* overexpression system and prepared the $^{113}Cd^{2+}$ bound SmtA with this system. With several NMR measurements (coupled with ^{15}N and ^{13}C labelling), we found that SmtA binds with 3 $^{113}Cd^{2+}$, and determined the solution structure of SmtA. On the basis of SmtA structure, we further designed multidomain-SmtAs, and measured the number of Zn^{2+}

bound with these proteins by ICP-AES, it was found that the numbers of Zn^{2+} bound with these proteins are in coincide with those planned. Furthermore, *E. coli* cells overexpressed these proteins accumulated the higher amounts of Zn^{2+} in the cell.

Structural studies for the C-terminal flexible region of telomere repeat binding protein, AtTRP-1 from *Arabidopsis Thaliana*.

S. Kojima and E.H. Morita
Proceedings of International Conference on Recent Innovations in Nanoscience & Technology 2019 (2020) 31–34.

Telomere is the characteristic nucleprotein structure located at the end of eukaryotic chromosomes, and indispensable for holding the gene structure during chromosome replication process. AtTRP-1 (578 AA) is one of the telomere-binding proteins found in *Arabidopsis thaliana*. This protein contains a Myb-like DNA binding domain (60 AA) recognizing telomere-repeat sequence and resembles with several initiator-binding proteins found in higher-plants. This Myb-like domain is followed by a C-terminal flexible region (55 AA). Previously, with Electro Mobility Shift Assaying (EMSA) technique, we have analyzed the binding affinities of the Myb-like domains followed by truncated C-terminal regions, to the model telomer repeat sequence. We have found that this Myb-like DNA binding domain, alone, does not have the ability to bind with telomere repeat sequence, and the presence of almost former half of the C-terminal flexible region is indispensable to sustain the native binding affinity to the telomere repeat sequence.

In this study, to clear the importance of the presence of the C-terminal region for the structural and functional stabilities of Myb-like domain, we have constructed the *E.coli* over-expression systems for 11 Myb-like domains with truncated C-terminal regions in different length and analyzed both the solubilities of overexpressed proteins, and the secondary structures with UV-CD measurements. We now compare the results for these structural analyses with those for previous EMSA, and will show the structural and functional importance of the C-terminal region, for the stability of Myb-like domain.

Axolotl as a model monitoring organism for water environment.

K. Mizuide and E. H. Morita
Proceedings of International Conference on Recent Innovations in Nanoscience & Technology 2019 (2020) 207–210.

As Amphibians spend almost of their life underwater, they are sensitive to water contamination. In particular, heavy metal is one of the most important water contamints not only for amphibians but also for mammalians including human being. To monitor water contamination by heavy metals, we have developed many ways, however, several problems still remain, such as the manufacturing cost for sensors, and the elctricity consumption, and establishing the

highly stable and sensitive amphibian system for monitoring water quality is an urgent need. To attain this, introducing the gene of fluorescent protein such as GFP, into the downstream of metallothionein gene is one way. For this gene edition, several techniques have been developed. Recently Crispr-Cas9 system is developed and it is much easier and highly reliable. With this technique, we planed to introduce GFP gene into the downstream of metallothionein gene. At now, as a model organism for amphibians, frogs (*Xenopus*) are usually used. However, this selection is based only on the relatively rapid development and salamanders including *Ambystoma mexicanum* (Axolotl) provide the better models for some aspects of vertebrate developments. In this point of view, we selected to use Axolotl as a model amphibian. To introduce Cas9-sgRNA complex into egg efficeintly at one cell stage, we now try to establish the elctropolation protcols as the easy, reliable and economical way for gene introduction to amphibian egg. In this presentation, we will show the results obtained until now.

Synthesis and characterization of Cu(I) isocyanide complexes exhibiting reversible luminescence

T. Hayakawa, C. Nanzan, M. Hashimoto, H. Teramae, T. Sakata
Jpn. J. Appl. Phys., **57**, (2018) 081601.

Herein, we describe the synthesis of Cu(I) isocyanide complexes, namely, the [CuI(PDI)] (PDI = 1,4-phenylene diisocyanide) dimer and $[Cu_2I_2(PPh_3)_2(PDI)_2]$ (PPh_3 = triphenylphosphine), which exhibit weak orange (quantum yield $\Phi = 1\%$) and intense pale blue ($\Phi = 13\%$) emissions in the solid state under UV irradiation, respectively. Upon grinding, the luminescence of the [CuI(PDI)] dimer does not change, whereas that of $[Cu_2I_2(PPh_3)_2(PDI)_2]$ changes to a weak olive ($\Phi = 4\%$) emission. Treatment of the ground $[Cu_2I_2(PPh_3)_2(PDI)_2]$ with an organic solvent and subsequent drying restore its original pale blue emission, which is indicative of reversible luminescent mechanochromism. Moreover, both the [CuI(PDI)] dimer and $[Cu_2I_2(PPh_3)_2(PDI)_2]$ exhibit thermochromism, i.e., their emissions change to a very intense green emission at 77 K. In particular, time-dependent density functional theory calculations reveal that $[Cu_2I_2(PPh_3)_2(PDI)_2]$ could be assigned to luminescence induced by halide-to-ligand charge transfer.

Reversible Formation of an Inter-molecular Compound Comprising 3′-Aminofluorene-9-spiro-5′-imidazolidine-2′,4′-dithione and Benzene

Y. Takazawa, T. Yamamoto, M. Suzuki, T. Sakata
Heterocycles, **96**, (2018) 2087–2095.

We herein describe the synthesis of 3′-aminofluorene-9-spiro-5′-imidazolidine-2′,4′-dithione through the reaction of fluorene-9-spiro-4′-thiazolidine-2′,5′-dithione with hydrazine, and subsequent investigation of the interactions of the synthesized spirocycle-containing imidazolidinedithione with organic solvents. Recrystallization from a solvent containing benzene led to

the formation of an inter-molecular compound consisting of 3′-aminofluorene-9-spiro-5′-imidazolidine-2′,4′-dithione and benzene in a 2:1 ratio through both intramolecular N-H···S hydrogen bonds and additional weak N-H···π interactions. The trapped benzene molecule was reversibly released by dissolution of the inter-molecular compound in acetone and subsequent concentration under reduced pressure at room temperature, and also by heating at 130–150 °C.

PVA Film Containing CuI Complex Exhibiting Mechanochromism

T. Sakata, C. Nanzan, Y. Takazawa
Proceedings of ICRINT2018, (2018) 255–259.

Herein, we describe the synthesis of a Cu(I)-iodide complex $[Cu_2I_2(DIB)_2(PPh_3)_2]$ (DIB = 1,4-diisocyanobenzene; PPh_3 = triphenylphosphine), which exhibits pale blue (Φ = 13%, λ_{max} = 474 nm) luminescence in the solid state under UV irradiation. Upon grinding, the luminescence of $[Cu_2I_2(PPh_3)_2(DIB)_2]$ changes to a weak olive (Φ = 4%) emission. Treatment of the ground $[Cu_2I_2(PPh_3)_2(DIB)_2]$ with an organic solvent (acetonitrile) and subsequent drying restore its original pale blue emission, which is indicative of reversible luminescent mechanochromism. $[Cu_2I_2(PPh_3)_2(DIB)_2]$ also exhibits thermochromism, i.e., the emission changes to a very intense green emission at 77 K (λ_{max} = 500 nm). In addition, $[Cu_2I_2(PPh_3)_2(DIB)_2]$ has two (temperature-dependent and temperature-independent) emission regions. The former was predominantly derived from the excimer based on the dipole-dipole interaction (Keesom force), which is expected to be fluorescent, whereas the latter, which is expected to be phosphorescent, corresponds to emission regardless of the Keesom energy. Moreover, time-dependent density functional theory (TD-DFT) calculations show that $[Cu_2I_2(PPh_3)_2(DIB)_2]$ could be assigned to luminescence induced by halide-to-ligand charge transfer (XLCT). Furthermore, we fabricated a polyvinyl alcohol (PVA) film containing $[Cu_2I_2(PPh_3)_2(DIB)_2]$ using a cast method and demonstrated reversible luminescent mechanochromism.

Reversible Luminescent Cu(I) Complex Exhibiting Mechanochromism

C. Nanzan, Y. Takazawa, M. Suzuki, H. Teramae, H. Miyamae, T. Sakata
Proceedings of ICRINT2018, (2018) 486–490.

Luminescent d^{10} complexes are attracting attention for application in post organic light-emitting diodes (OLEDs) as they drastically suppress non-radiative deactivation, due to the absence of d-d transitions. In particular, Cu(I) complexes have received increased attention because they show strong emission and are based on copper, which is relatively inexpensive and abundant. Among them, the Cu(I)-halide complexes are well known for their structurally rich photophysical behavior and high luminescence efficiency. Some of these complexes exhibit luminescent color changes due to external stimuli. Here, a Cu(I)-bromide complex is investigated to develop a high-efficiency complex with luminescent mechanochromism for optical and physical applications. $[Cu_4Br_4(PPh_3)_4]$, obtained by stirring copper (I)

bromide (CuBr) and triphenylphosphine (PPh_3), reacts with 1,4-diisocyanobenzene (DIB) to form $[Cu_2Br_2(DIB)_2(PPh_2)_2]_n$. The resulting complex showed bluish green (λ_{max} = 498 nm) and green (λ_{max} = 515 nm) emission at 295 and at 77 K, respectively. TD-DFT calculations reveal that the emission corresponding to the high-energy (HE) and low-energy (LE) bands is due to (halogen+metal)-to-ligand and halogen-to-ligand charge transfers ((X+M) LCT and XLCT). Also, mechanical stimuli, such as grinding, causes color changes similar to temperature stimuli. The finely crushed complex returns to the initial bluish green emission after being dipped into acetonitrile and then evaporating the solvent, demonstrating reversible luminescent color. The behavior of the powder X-ray diffraction (PXRD) patterns suggests that the change in luminescent color is related to the crystal-to-amorphous phase conversion.

Aromatic Structures Trapped by Molecular Compounds Comprising 3′-Aminofluorene-9-spiro-5′-imidazolidine-2′,4′-dithione

T. Sakata, C. Nanzan, Y. Takazawa, T. Yamamoto
Proceedings of ISENT2019, (2019) 295–299.

Derivatives of imidazolidine-2-thione are promising biologically and pharmacologically active molecules. 3′-Aminofluorene-9-spiro-5′-imidazolidine-2′,4′-dithione (HM1) which is synthesized by the reaction of fluorene-9-spiro-4′-thiazolidine-2′,5′-dithione with hydrazine (T. Yamamoto, et al., J. Chem. Soc. Perkin Trans. 1, 1990, 3003), forms a molecular compound with benzene in a ratio of 2:1. Also, HM1 desorbs trapped benzene by heating or immersing into polar solvents (Y. Takazawa, et al., Heterocycles, 2018, 96, 2087). Herein, planar and non-planar aromatic solvents were investigated to validate the chemical structure of trapped molecules. Yellow microcrystalline structure were obtained after dis-solving HM1 and evaporating the aromatic solvents. Using pyrrole or thiophene, IR absorption peaks from the N-H or C-S stretching vibration of pyrrole or thiophene appeared in the MC1 spectra, indicating the presence of pyrrole or thiophene molecules in the microcrystalline material. After heating under vacuum at 70 °C for 7 h, there was no change in the corresponding IR adsorption peaks, showing that HM1 forms a compound containing pyrrole or thiophene, as was shown for benzene as a trapped molecule. On the other hand, no IR peaks were detected for both toluene or p-xylene in the microcrystal-line structure, confirming that HM1 does not form a molecular compound with them. Therefore, HM1 forms a molecular compound with planar molecules but not with non-planar molecules, which is due to the steric hindrance of the alkyl-substituent.

Luminescent Properties of a polymeric copper (I)-bromide complex in a PMMA film

C. Nanzan, Y. Takazawa, M. Suzuki, H. Teramae, T. Sakata
Jpn. J. Appl. Phys., **59**, (2020) 077001.

The $[Cu_2Br_2(DIB)_2(PPh_2)_2]_n$ complex, obtained by the reaction between $[Cu_4Br_4(PPh_3)_4]$

and 1,4-diisocyanobenzene (DIB), was found to have a bridged polymeric structure with a planar $\{Cu_2Br_2\}$ core. The compound exhibited bluish-green (λmax = 498 nm) and green (λmax = 515 nm) luminescence at 295 and 77 K, respectively, corresponding to the emissions from XLCT (HE band) and (X+M) LCT (LE band), respectively. The dual emission, which is attributed to the luminescence from both bands, was observed at around 178 K. The complex also displayed a change in luminescence color from bluish-green to yellow (λmax = 529 nm) upon applying external mechanical stimuli. The film containing $[Cu_2Br_2(DIB)_2(PPh_2)_2]$ n was prepared by a cast method using polymethyl methacrylate as a binding agent. The rubbed part of the film turned yellow and the other parts maintained bluish-green luminescence. Restoration of the initial color was feasible by annealing, even in film state.

Cocrystals of Li^+ encapsulated fullerenes and Tb (iii) double-decker single molecule magnet in a quasi-kagome lattice

H. Iwami,[*1] J. Xing,[*1] R. Nakanishi,[*1] Y. Horii,[*1] K. Katoh,[*1] B. K. Breedlove,[*1] K. Kawachi,[*2] Y. Kasama,[*2] E. Kwon,[*1] M. Yamashita[*1,3] (*1 Tohoku University, *2 Idea International Co. Ltd. *3 Nankai University)
Chemical Communications, **56,** (2020) 12785-12788 .

Cocrystallization of a Li^+ ion encapsulated fullerene $Li^+@C_{60}$ with a Tb^{3+} phthalocyaninato porphyrinato double-decker single-molecule magnet [Tb (Pc) (OEP)] is reported. The cocrystal, packs in a quasi-kagome lattice, which leads to intermolecular ferromagnetic interactions as well as the modulation of the single-molecule magnet properties.

Highly oxidized states of phthalocyaninato terbium (III) multiple-decker complexes showing structural deformations, biradical properties and decreases in magnetic anisotropy

Y. Horii,[*1] M. Damjanović,[*2,7] M. R. Ajayakumar,[*3] K. Katoh,[*1] Y. Kitagawa,[*4] L. Chibotaru,[*5] L. Ungur,[*6] M. Mas-Torrent,[*3] W. Wernsdorfer,[*7] B. K. Breedlove,[*1] M. Enders,[*2] J. Veciana,[*3] M. Yamashita[*1,8] (*1 Tohoku University, *2 Heidelberg University, *3 Institut de Ciencia de Materials de Barcelona, *4 Osaka University, *5 Katholieke Universiteit Leuven, *6 National University of Singapore, *7 Karlsruhe Institute of Technology, *8 Nankai University)
Chemistry European Journal, **26**, (2020) 8621-8630.

Presented here is a comprehensive study of highly oxidized multiple-decker complexes composed of Tb^{3+} and Cd^{2+} ions and two to five phthalocyaninato ligands, which are stabilized by electron-donating n-butoxy groups. Magnetic measurements revealed that the series of complexes show single-molecule magnet properties, which are controlled by the multi-step redox induced structural changes.

Coexistence of Spin-Lattice Relaxation and Phonon-Bottleneck Processes in GdIII-Phthlocyaninato Triple-Decker Complexes under Highly Diluted Conditions

Y. Horii,[*1] K. Katoh,[*1] Y. Miyazaki,[*2] M. Damjanović,[*3] T. Sato,[*1] L. Ungur,[*4] L. F. Chibotaru,[*5] B. K. Breedlove,[*1] M. Nakano,[*2] W. Wernsdorfer,[*3] M. Yamashita[*1,6] (*1 Tohoku University, *2 Osaka University, *3 Karlsruhe Institute of Technology, *4 National University of Singapore, *5 Katholieke Universiteit Leuven, *6 Nankai University)
Chemistry European Journal, **26**, (2020) 8076-8082.

Gadolinium (III) (Gd^{3+}) complexes have been shown to undergo unusual slow magnetic relaxation processes similar to those of single-molecule magnets (SMMs), even though Gd^{3+} does not exhibit strong magnetic anisotropy. It was found that the Gd^{3+}-Gd^{3+} interactions accelerate the magnetic relaxation processes. A detailed dynamic magnetic analysis revealed that the coexistence of spin-lattice relaxation and phonon-bottleneck processes is the origin of the dual magnetic relaxation processes.

Manipulation of the Magnetic Anisotropy along the C_4 Rotation Axis via a Supramolecular Approach

K. Katoh,[*1] N. Yasuda,[*2] M. Damjanović,[*3] W. Wernsdorfer,[*3] B. K. Breedlove,[*1] M. Yamashita[*1,4] (*1 Tohoku University, *2 Japan Synchrotron Radiation Research Institute, *3 Karlsruhe Institute of Technology, *4 Nankai University)
Chemistry European Journal, **26**, (2020) 4805-4815.

A supramolecular complex was prepared by assembling C_{60} with the dinuclear Tb^{3+} triple-decker complex [(TPP)Tb(Pc)Tb(TPP)] with quasi-D_{4h} symmetry to investigate the relationship between the coordination symmetry and single-molecule magnet (SMM) properties. From temperature and magnetic field dependences of τ, spin-phonon interactions along with direct and Raman mechanisms explain the spin dynamics. We believe that a supramolecular method can be used to control the magnetic anisotropy along the C_4 rotation axis and the spin dynamic properties in dinuclear Tb^{3+}-Pc multiple-decker complexes.

Simultaneous Spin-Crossover Transition and Conductivity Switching in a Dinuclear Iron (II) Coordination Compound Based on 7,7′ ,8,8′ -Tetracyano-p-quinodimethane

R. Ishikawa,[*1] S. Ueno,[*1] S. Nifuku,[*1] Y. Horii,[*2] H. Iguchi,[*3] Y. Miyazaki,[*2] M. Nakano,[*2] S. Hayami,[*4] S. Kumagai,[*5] K. Katoh,[*3] Z-Y. Li,[*6] M. Yamashita,[*3,6] S. Kawata[*1] (*1 Fukuoka University, *2 Osaka University, *3 Tohoku University, *4 Kumamoto University, *5 The University of Tokyo, *6 Nankai University)
Chemistry European Journal, **26**, (2020) 1278-1285.

The reaction of Fe $(OAc)_2$ and Hbpypz with neutral TCNQ results in the formation of

$[Fe_2(bpypz)_2(TCNQ)_2](TCNQ)_2$ (**1**). Temperature dependence of the dc magnetic susceptibility and heat capacity measurements indicate that **1** undergoes an abrupt spin crossover (SCO) with thermal spin transition temperatures of 339 and 337 K for the heating and cooling modes, respectively, resulting in a thermal hysteresis of 2 K. Remarkably, the temperature dependence of dc electrical transport exhibits a transition that coincides with thermal SCO, demonstrating the thermally induced magnetic and electrical bistability of **1**, strongly correlating magnetism with electrical conductivity.

Reaction of C_{60} radical anion with alkyl halide

Y. Maeda[*1], M. Sanno[*1], T. Morishita[*1], K. Sakamoto[*1], E. Sugiyama[*1], S. Akita[*1], M. Yamada[*1], M. Suzuki (*1 Tokyo Gakugei University)
New J. Chem. **43**, (2019) 6457–6460.

The reaction of the C_{60} radical anion with *a*-bromo-1,3-dicarbonyl compounds selectively afforded the methanofullerene derivatives. The reaction with 1,2-bis (dihalomethyl)-benzene and benzyl halide afforded the corresponding 1,4-dibenzylated C_{60} derivative and cycloaddition product, respectively. The possible mechanisms for the formation of the fullerene adducts via electron transfer are proposed.

Synthesis of Fullerene-Fluorene Dyads through the Platinum-Catalyzed Reactions of [60] Fullerene with 9-Ethynyl-9H-fluoren-9-yl Carboxylates

M. Yamada[*1], M. Takizawa[*1], Y. Nukatani[*1], M. Suzuki, and Y. Maeda[*1] (*1 Tokyo Gakugei University)
J. Org. Chem. 84, (2019) 9025–9033.

The single-step regio- and stereo-selective platinum-catalyzed reactions of C_{60} with a series of 9-ethynyl-9*H*-fluoren-9-yl carboxylates afforded C_{60}-fluorene dyads in their [2+2] cycloaddition. The presented reactions represent the first examples of the use of easily accessible fluorenyl carboxylates as fluorenylideneallene precursors. In addition, the single-crystal X-ray structure of one of the dyads shows a distorted cyclobutane ring. Furthermore, the dyad forms a layered structure with close-packed arrays of C_{60} in its crystals.

Sonochemical reaction to control the near-infrared photoluminescence properties of single-walled carbon nanotubes

Y. Maeda[*1], Y. Konno[*1], A. Nishino[*1], M. Yamada[*1], S. Okudaira[*2], Y. Miyauchi[*2], K. Matsuda[*2], J. Matsui[*3], M. Mitsuishi[*4], and M. Suzuki (*1 Tokyo Gakugei University, *2 Kyoto University, *3 Yamagata University, *4 Tohoku University)
Nanoscale, *12*, (2020) 6263–6270.

The effect of ultrasonic irradiation on the optical properties of single-walled carbon nanotubes (SWNTs) was studied. Upon sonication in deuterated water in the presence of sodium dodecylbenzene sulfonate under air, red-shifted photoluminescence peaks at ~1043 and ~1118 nm were observed from the aqueous suspensions of (6,4) and (6,5) SWNTs, accompanied by a decrease in the intensity of the intrinsic photoluminescence peaks. Upon sonication with sodium dodecylbenzene sulfonate under an Ar atmosphere, the rate of spectral change increased with the sonication time and new photoluminescence peaks emerged at 1043, 1118, and 1221 nm. Meanwhile, upon the addition of 1-butanol, the photoluminescence peaks emerged only at 1043 nm and 1118 nm, while the emergence of the peak at 1221 nm was inhibited. On the other hand, a suspension with highly dispersed SWNTs was obtained upon sonication in the presence of sodium cholate without any change in the intrinsic optical properties of SWNTs. These experimental results elucidate that the photoluminescence characteristics of SWNTs can be controlled by controlling the sonication conditions such as the type of surfactant used, the concentration of SWNTs, reaction environment, and the presence of an inhibitor such as 1-butanol.

Syntheses and crystal structures of two piperine derivatives

T. Ezawa[*1], Y. Inoue[*1], I. Murata[*1], M. Suzuki, K. Takao[*1], Y. Sugita[*1], I. Kanamoto[*1] (*1 Faculty of Pharmacy and Pharmaceutical Science, Josai University)
Acta cryst. E76, (2020) 646-650.

The title compounds, 5-(2*H*-1,3-benzodioxol-5-yl)-*N*-cyclohexylpenta-2,4-diena-mide (I), and 5-(2*H*-1,3-benzodioxol-5-yl)-1-(pyrrolidin-1-yl) penta-2,4-dien-1-one (II) are derivatives of piperine, which is known as a pungent component of pepper. Their geometrical parameters are similar to those of the three polymorphs of piperine, which indicate conjugation of electrons over the length of the molecules. The extended structure of compound I features amide hydrogen bonds, which generate $C(4)$ [010] chains. The crystal of compound II features aromatic π-π stacking, as for two of three known piperine polymorphs.

Copper-Mediated Cascade Synthesis of Open-Cage Fullerenes

M. Yamada[*1], A. Ishitsuka[*1], Y. Maeda[*1], M. Suzuki, H. Sato[*2] (*1 Tokyo Gakugei University, *2 Rigaku Corporation)
Org. Lett. 22, (2020) 3633-3636.

An open-cage fullerene having an eight-membered ring orifice has been synthesized in one-pot by the reaction of [60] fullerene with propargylic phosphate in the presence of CuCl. The reaction cascade includes the transformation of the phosphate to the 1,3-dienyl phosphate, which enables the reaction with [60] fullerene by [4+2] cycloaddition to form the cyclohexene-annulated intermediate, and subsequent intramolecular syn-elimination of the phosphodiester affords the cyclohexadiene-annulated fullerene derivative as the precursor for

the open-cage fullerene.

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組み～平成 23-25 年度

北川浩子
城西大学　教職課程センター紀要．**3**, 81-84（3 月 2019）

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が示唆された。

川越市「小・中・大学連携理科ふれあい事業」への取り組み

宇和田貴之，石黒直哉，北川浩子[†]
城西大学　教職課程センター紀要．**3**, 85-90（3 月 2019）

川越市が市内の小・中学生の理科に対する興味・関心や知的好奇心，探究心を醸成するため毎年度開催している川越市「小・中・大学連携理科ふれあい事業」では，川越市近隣大学の教員および学生を小・中学校に招き，理科に関する実験・実習を行っている。本学理学部化学科の教員は本事業に継続的に参加し貢献している。本稿では 2016 ～ 2017 年度の我々の本事業への取り組み内容を報告し，理学部教員としての地域への貢献のあり方を考察する。

Habitat of a native freshwater shrimp *Paratya improvisa* in Iruma River system in Saitama Prefecture and the invasion status of alien species, *Neocaridina* spp

N. Ishiguro, N. Tamura, M. Ohkashiwa
DNA 鑑定，**10**, 51-58（2018）

Paratya improvisa is a freshwater shrimp species indigenous to eastern Japan. Originally, no species of the genus *Neocaridina* inhabited this region, however, invasion by *Neocaridina* species has been confirmed in Shiga, Kanagawa, Chiba, Miyagi Prefectures and Hokkaido. In this study, the mitochondrial DNA analysis of cytochrome oxidase subunit I gene demonstrated that *Neocaridina* species have invaded almost all areas within Saitama Prefecture. The presence of indigenous *P. improvisa* was observed in only two areas in the upper river basins. Our findings indicate that the prevalence of *Neocaridina* species increases further downstream within the same river system. In addition, *Neocaridina* species have also adapted to irrigation canals and other environments containing less water.

環境 DNA を用いたアベサンショウウオ（*Hynobius abei*）の分布とその生息域におけるアメリカザリガニの侵入調査

日和佳政[*1]，藤長裕平[*1]，鈴木裕士，矢島美貴，石黒直哉（*1 越前市産業環境部）
DNA 多型，**27**, 1-8 (2019).

Environmental DNA (eDNA) requires less time and effort compared to traditional surveys to detect species. Many habitat surveys, there, can be applicable using eDNA. Here we developed new PCR primer pairs for eDNA method to monitor Japanese endangered salamander, *Hynobius abei*. Also, invasion of American crayfish that preys on salamander is confirmed at several sites where *H. abei* habitats. Therefore, we designed PCR primer sets to detect American crayfish invasion to *H. abei* habitats. This eDNA method was carried out using water samples collected from eight habitats of *H. abei*. The eDNA method detected five habitats of *H. abei* in the western area of Echizen Fukui. In addition, the eDNA method revealed crayfish invasion in 8 *H. abei* habitats of 23 habitats we surveyed. We conclude that the eDNA method is a powerful tool for the monitoring *H. abei*, and crayfish invasion to *H.abei* habitats.

ミトコンドリア DNA 調節領域の塩基配列分析によるヤマノカミの遺伝的多様性

石黒直哉，藤田健太郎，田原大輔[*1]，竹下直彦[*2]（*1 福井県大，*2 水大校）
DNA 鑑定，**11**, 31-39 (2019).

The roughskin sculpin, Trachidermus fasciatus (Scorpaeniformes：Cottidae), is distributed in Japanese, Chinese, and Korean coastlines and the rivers flowing into these water bodies. The roughskin sculpin has a catadromous life history：spawning occurs around the shallow mudflats of the bay, and the larvae ascend upstream of the major rivers. Here we investigated the genetic diversity of the roughskin sculpin using nucleotide sequence data from the mitochondrial control region (715 bp) of 86 individuals collected from 12 rivers in the Ariake Bay. In total, 10 haplotypes were observed from 13 permutation sites. The most dominant haplotype was shared by 11 rivers. However, the haplotype network did not show a star-like shape. The haplotype and nucleotide diversities were 0.838 and 0.00589, respectively. The estimate of pairwise F ST did not show a significant difference in nine out of the 10 populations. The estimated divergence time for the Japanese and Chinese populations was much greater than that expected for the apparently relictual population distributed in the Ariake Bay.

Male parental assistance in embryo hatching of barred-chin blenny *Rhabdoblennius nitidus*.

Kaori Sano, Risa Yokoyama, Takako Kitano[*1], Takeshi Takegaki[*1], Nobumasa Kitazawa, Toyoji Kaneko[*2], Yoshihide Nishino[*3], Shigeki Yasumasu[*3], Mari Kawaguchi[*3] (*1 Nagasaki University, *2 The University of Tokyo, *3 Sophia University)
J Exp Zool B Mol Dev Evol, **332**, 81-91 (2018)

Most teleostean embryos develop and hatch without parental assistance, though some receive parental care. We focused on a paternal brood-care species, the barred-chin blenny *Rhabdoblennius nitidus*. We analyzed genes for the hatching enzyme and egg-envelope protein, which were successfully cloned from barred-chin blenny, and found the expression patterns differed from those of other euteleosts. Our study illustrates an example of the evolution of parent-embryo interaction built on a novel relationship: Degradation of the hatching enzyme/egg-envelope digestion system, accompanied by male parental hatching assistance.

Mother-to-embryo vitellogenin transport in a viviparous teleost *Xenotoca eiseni*.

Atsuo Iida[*1], Hiroyuki N Arai[*2], Yumiko Someya[*3], Mayu Inokuchi[*3], Takeshi A Onuma[*4], Hayato Yokoi[*5], Tohru Suzuki[*5], Eiichi Hondo[*1], Kaori Sano（∗1 Nagoya University, ∗2 Kyoto University, ∗3 Toyo University ∗4 Osaka University, ∗5Tohoku University）
PNAS, **116**, 22359-22365（2019）

Vitellogenin（Vtg）, a yolk nutrient protein that is synthesized in the livers of female animals, and subsequently carried into the ovary, contributes to vitellogenesis in oviparous animals. In this study, we identified Vtg protein in the livers of females during the gestation of the viviparous teleost, *Xenotoca eiseni* Although vitellogenesis is arrested during gestation, biochemical assays revealed that Vtg protein was present in ovarian tissues and lumen fluid. Our data suggest that the yolk protein is one of the matrotrophic factors supplied from the mother to the intraovarian embryo during gestation in *X. eiseni*.

In Situ absorption and fluorescence microspectroscopy investigation of the molecular incorporation process into single nanoporous protein crystals

Takayuki Uwada, Kohei Kouno, and Mitsuru Ishikawa
ACS Omega, **5**, 9605-9613（2020）.

Protein crystals exhibit distinct three-dimensional structures, which contain well-ordered nanoporous solvent channels, providing a chemically heterogeneous environment. In this paper, the incorporation of various molecules into the solvent channels of native hen egg-white lysozyme crystals was demonstrated using fluorescent dyes, including acridine yellow G, rhodamine 6G, and eosin Y. The process was evaluated on the basis of absorption and fluorescence microspectroscopy at a single-crystal level. The molecular loading process was clearly visualized as a function of time, and it was determined that the protein crystals could act as nanoporous materials. It was found that the incorporation process is strongly dependent on the molecular charge, leading to heterogeneous molecular aggregation, which suggests host-guest interaction of protein crystals from the viewpoint of nanoporous materials.

Liquid-liquid interface can promote micro-scale thermal Marangoni convection in liquid binary mixtures

Issei Aibara*, Tatsuki Katoh*, Chihiro Minamoto*, Takayuki Uwada, Shuichi Hashimoto* (* Department of Optical Science and Technology, University of Tokushima)
J. Phys. Chem. C, **124**, 2427–2438 (2020).

Liquid-liquid phase separation, a physical transition in which a homogeneous solution spontaneously demixes into two coexisting liquid phases, has been a key topic in the thermodynamics of two-component systems and may find applications in separation, drug delivery, and protein crystallization. Here we applied a microscale temperature gradient using optothermal heating of a gold nanoparticle to overcome the experimental difficulties inherent in homogeneous heating: We aimed at highlighting precise structural development by avoiding randomly nucleating/growing microdomains. In response to laser illumination, a single gold nanoparticle immersed in a binary mixture of aqueous 2,6-dimethylpyridine (lutidine) and N-isopropylpropionamide (NiPPA) was clearly sensitive to the phase transition of the surrounding liquid as demonstrated by light-scattering signals: spectral red-shifts and bright-spot images. The local phase separation encapsulating the gold nanoparticle resulted in immediate formation and growth of an organic-rich droplet which was confirmed by Raman spectroscopy. Remarkably, the droplet was stable under a nonequilibrium steady-state heating condition because of strong thermal confinement. Microdroplet growth was ascribed to thermocapillary flow induced by a newly formed liquid-liquid interface around the hot gold nanoparticle. On the basis of a tracer experiment and numerical simulation, it is deduced that the transport of solute to the high-temperature area is driven by this thermocapillary flow. This study enhances our understanding of phase separation in binary mixtures induced by microscale temperature confinement.

Flow-induced transport via optical heating of a single gold nanoparticle

Jun-ichi Chikazawa*, Takayuki Uwada, Akihiro Furube*, and Shuichi Hashimoto* (* Department of Optical Science and Technology, University of Tokushima)
J. Phys. Chem. C, **123**, 4512–4522 (2019).

Optothermal trapping has gained increasing popularity in manipulation such as selecting, guiding, and positioning submicron objects because of a few mW laser power much lower than that required for optical trapping. Optothermal trapping uses thermal-gradient-induced phoretic motions, but the underlying physics of driving force has not been fully understood. In this study, we performed optothermal trapping of 500 nm-diameter colloidal silica via a continuous laser illumination of a single gold nanoparticle from the bottom in a closed chamber. Under illumination, the tracer particles were attracted to the gold nanoparticle and trapped. Notably, the direction of migrating particles was always to hot gold nanoparticles regardless of the configuration of gold nanoparticles placed at two opposite sides of the chamber, on

the bottom surface of an upper substrate (ceiling) or on the top surface of a lower substrate (floor). The previous interpretation based on thermal convective flow from the bottom to the top and circulating inside the chamber was only applicable to floor configuration and failed to explain our observation for the ceiling. Instead, temperature-induced Marangoni effect at the water/superheated water interface is likely to play a role. This study promoted a better understanding of the driving mechanism in optothermal trapping. Moreover, as an application of the single-particle platform, we showed the photothermal phase separation-induced microdroplet formation of thermoresponsive polymers and the coating of non-thermoresponsive polymers on nanoparticles.

In Vitro Anti-tumor Activity of Alkylaminoguaiazulenes

Mari Uehara, Himawari Minemura, Tunenori Ohno, Masashi Hashimoto, Hidetsugu Wakabayashi, Noriyuki Okudaira[*1], and Hiroshi Sakagami[*1] (*1 Department of Endodontics, Meikai University)
International Journal of In Vivo Research, **32**, No.3, 541-547 (2018).

We investigated the relative cytotoxicity of 10 alkylaminoguaiazulene derivatives towards both cancer and normal cells. Tumor specificity (TS) was evaluated as the ratio of the mean 50% cytotoxic concentration against normal oral cells to that against OSCC cell lines. Apoptosis-inducing activity was evaluated by cleavage of poly ADP-ribose polymerase and caspsase-3 with western blot analysis. Validity of the present TS measurement method was confirmed using methotrexate. With increasing length of the alkyl group of alkylaminoguaiazulene derivatives, cytotoxicity increased. Introduction of oxygen, nitrogen or sulfur atom into the alkyl group slightly reduced cytotoxicity. Most compounds had very low TS, no synergistic action with methotrexate and doxorubicin, nor did they induce apoptosis of OSCC cells.

Quantitative Structure-Cytotoxicity Relationship of Azulene Amide Derivatives

Kana Imanari, Masashi Hashimoto, Hidetsugu Wakabayashi, Noriyuki Okudaira[*1], Kenjiro Bandow[*1], Junko Nagai[*1], Mineko Tomomura[*1], Akito Tomomura[*1], Yoshihiro Uesawa[*2] and Hiroshi Sakagami[*1] (*1 Department of Endodontics, Meikai University, *2 School of Dentistry Department of Clinical Pharmaceutics, Meiji Pharmaceutical University)
Anticancer Res., **39**, 3507-3518 (2019).

Very few studies of anticancer activity of azulene amides led us to investigate the cytotoxicity of 21 *N*-alkylazulene-1-carboxamides introduced either with 3-methyl, 7-isopropyl-3-methyl or 2-methoxy derivatives. Tumorspecificity (TS) was calculated by the ratio of mean 50% cytotoxic concentration (CC_{50}) against three normal human oral mesenchymal cells to that against four human oral squamous cell carcinoma (OSCC) cell lines. Potencyselectivity expression (PSE) was calculated by dividing TS value by CC_{50} value against OSCC cell lines. Apoptosisinducing activity was evaluated by caspase-3 activation and appearance

of subG1 cell population. 7-Isopropyl-3-methyl derivatives showed higher TS and PSE values, than 3-methyl derivatives and 2-methoxy derivatives. The most active 7-isopropyl-3-methyl derivatives induced apoptosis in C9-22 OSCC cells at 4-times higher CC_{50}. Quantitative structure-activity relationship analysis of 3-methyl derivatives and 7-isopropyl-3-methyl derivatives demonstrated that their tumorspecificity was correlated with chemical descriptors that explain the molecular shape and hydrophobicity. 7-Isopropyl-3-methyl-*N*-propylazulene-1-carboxamide can be a potential candidate of lead compound for manufacturing new anticancer drug.

Antitumor Effects and Tumor-specificity of Guaiazulene-3-Carboxylate Derivatives Against Oral Squamous Cell Carcinoma In Vitro

Michihito Teratani, Shouta Nakamura, Hiroshi Sakagami[*1], Masakazu Fujise, Masashi Hashimoto, Noriyuki Okudaira[*1], Kenjiro Bandow[*1], Yoseke Iijima[*2], Junko Nagai[*3], Yoshihiro Uesawa[*3] and Hidetsugu Wakabayashi (*1 Department of Endodontics, Meikai University, *2 Department of Oral and Maxillofacial Surgery, Saitama Medical University, *3 School of Dentistry Department of Clinical Pharmaceutics, Meiji Pharmaceutical University)
Anticancer Res., **40**: 4885-4894 (2020).

The aim of this study was to investigate the antitumor potential of guaiazulene-3-carboxylate derivatives against oral malignant cells. Twelve guaiazulene-3-carboxylate derivatives were synthesized by introduction of either with alkyl derivatives, alkoxy derivatives, hydroxyl derivatives or primary amine derivatives at the end of sidechains. Tumor-specificity (TS) was calculated by the ratio of mean 50% cytotoxic concentration (CC_{50}) against 3 human oral mesenchymal cell lines to that against 4 human oral squamous cell carcinoma (OSCC) cell lines. Potencyselectivity expression (PSE) was calculated by dividing TS value by CC_{50} value against OSCC cell lines. Cell cycle analysis was performed by cell sorter. Alkoxy derivatives showed the highest TS and PSE values, and induced the accumulation of both subG1 and G2/M cell populations in HSC-2 OSCC cells. Quantitative structure-activity relationship analysis demonstrated that their tumor-specificity was correlated with chemical descriptors that explain the 3D shape, electric state and ionization potential.

Preparation, characterization, and study of the antimicrobial activity of a Hinokitiol-copper(II)/γ-cyclodextrin ternary complex.

R. Suzuki, Y. Inoue*, I. Murata, H. Nomura, Y. Isshiki, M. Hashimoto, Y. Kudo, H. Kitagishi, S. Kondo,I. Kanamoto. (* Faculty of Pharmacy and Pharmaceutical Sciences, Josai University)
Journal of Molecular Structure, **1194**, 19-27 (2019).

The aim of the current study was to prepare a ternary complex of hinokitiol (HT), a metal ion (Cu (II)) and g-cyclodextrin (gCD) via coprecipitation and to assess its physicochemical properties and the effects of complexation on the antimicrobial activity of HT.

The antimicrobial action of HT can presumably be capitalized on by including HT in CD without a metal in certain applications. The current results should provide a basis for use of hinokitiol as a human and environmentally friendly antimicrobial.

Metal-Dependent DNA Base Pairing of 5-Carboxyuracil with Itself and All Four Canonical Nucleobases

Yusuke Takezawa,[*1] Akira Suzuki,[*1] Manabu Nakaya, Kotaro Nishiyama[*1] and Mitsuhiko Shionoya[*1] (∗1 The University of Tokyo) *J. Am. Chem. Soc.* **142,** 21640-21644 (2020).

A 5-carboxyuracil (caU) nucleobase was found to pair not only with A (caU-A) by hydrogen bonding but also withother DNA nucleobases by metal coordination bonding. Metal-dependent formation of caU-Cu^{II}-caU, caU-Hg^{II}-T, caU-AgI-C, and caU-Cu^{II}-G pairs was demonstrated by duplex melting analysis and mass spectrometry. The duplexes containing caU-X (X = caU, T, C, and G) were significantly stabilized in the presence of the corresponding metal ions, while the DNA duplexes containing the caU-A pairs were destabilized by the addition of Cu^{II}. These results suggest that the hybridization partner of caU-containing DNA strands can be altered by metal complexation. As a result, this study provides a new direction to integrate caU nucleobases to construct diverse metallo-DNA supramolecules and metal-responsive DNA devices.

CO_2-Induced Spin-State Switching at Room Temperature in a Monomeric Cobalt (II) Complex with the Porous Nature

Manabu Nakaya, Wataru Kosaka,[*1] Hitoshi Miyasaka,[*1] Yuki Komatsumaru,[*2] Shogo Kawaguchi,[*3] Kunihisa Sugimoto,[*3] Yingjie Zhang,[*4] Masaaki Nakamura,[*2] Leonard F. Lindoy[*5] and Shinya Hayami[*2] (∗1 Tohoku University, ∗2 Kumamoto University, ∗3 JASRI, ∗4 ANSTO, ∗5 The University of Sydney)
Angew. Chem. Int. Ed. **59**, 10658-10665 (2020).

The first example of CO_2-responsive spin state conversion between high-spin (HS) and low-spin (LS) states at room temperature was achieved in a monomeric cobalt (II) complex. A neutral cobalt (II) complex, $[Co^{II}(COO\text{-terpy})_2] \cdot 4H_2O$ (**1·4H$_2$O**), stably formed cavities generated via π-π stacking motifs and hydrogen bond networks, resulted in the accommodation of four water molecules. A crystalline **1·4H$_2$O** transformed to the solvent-free **1** without loss of the porosity by heating up to 420 K. Compound **1** exhibited a selective carbon dioxide (CO_2) adsorption via a gate-open type of the structural modification. Furthermore, the HS/LS transition temperature ($T_{1/2}$) was able to be tuned by the CO_2-pressure over a wide temperature range. Unlike **1** exhibits the HS state at 290 K, the CO_2-accomodated form **1 ⊃ CO$_2$** (P_{CO2} = 110 kPa) was stabilized in the LS state at 290 K probably caused by "chemical pressure" effect by CO_2 accommodation, which provides reversible spin-state conversion by introducing/evacuating CO_2 gas into/from **1**. This result represents an important advance providing new

insights for the development of new gas-responsive functional magnetic materials in the future.

Guest Modulated Spin States of Metal Complex Assemblies

Manabu Nakaya, Ryo Ohtani[*1] and Shinya Hayami[*2] (*1 Kyushu University, *2 Kumamoto University)
Eur. J. Inorg. Chem., **2020**, 3709–3719 (2020) (mini review).

Recently, "host-guest chemistry" aspects of material science have received much attention, particularly in relation to moderating the functions of materials. In particular, magnetic properties involving the "magnetic ordering" and "spin cross-over" of host-guest metal complex systems have been actively investigated in terms of their host-guest chemistry. That is, systems in which the magnetic properties are sensitive to perturbation by the uptake of guests (which thus act as chemical stimuli). Such guests (solvents, gases and organic molecules) very often influence the structures of both discrete metallo-supramolecular assemblies as well as those of coordination polymers/metal-organic frameworks (CPs/MOFs), providing a means for fine-tuning their magnetic behavior, including the switching of their spin states. In this minireview, we report recent progress in the development and investigation of magnetic materials of both the CP and MOF categories as well as of discrete complexes whose properties are modulated by guests

Thermal Stability of Piezoelectric Materials at High Temperature

Thithi Lay
Proceedings of the International Symposium on Environmental-Life Science and Nanoscales Technology 2019 (ISENT2019) 378–381 (2019)

Piezoelectric sensors and actuators are widely used in sensing applications such as vehicle high pressure monitoring system, diesel engine sensing, airplane engine monitoring system, etc. These applications are operated under extreme conditions such as high temperature, low temperature, high pressure, and high electric field.

This research work focused on measurement method and device properties under high temperature as a function of time. Electromechanical coupling factor ((Kp) which is important for energy conversion from electrical properties to mechanical properties and vice versa is calculated and compared at various temperature. To achieve precise values of electromechanical coupling factor we used measurement protocol which is stated in JIS (R1699-12016) and carried out the experiment according to the protocol. Calculated electromechanical factor for both multilayer and round disk piezoelectric materials from room temperature to 160℃. From the results of calculated electromechanical coupling factor (Kp) present measurement protocol might be able to apply as differential thermal analysis method for material and device properties under high temperature.

Spectral Analysis of Transition Metal Carbides for Sustainable Industrial Development

Thithi Lay, M. Imamura[*1], N. Matsubayashi[*1], M. Jo[*1], Khin Khin Win [*2] (*1 National Institute of *Advanced Industrial Science and Technology* (*AIST*), *2 University of Yangon)
Proceedings of the 19th. Science Council of Asia (*SCA*) *Conference,* (*Research and Innovation for Sustainable Development in Asia,* 2019) 53.4,1-6 (2019)

Development of transition metals carbides (T-M-C) in industrial become importance due to its unique properties such as hardness, metal conductivity and high temperatures capability [1,2]. There have been widespread in applications of T-M-C compounds as catalysis, hard coatings, wear-resistant components and electron emitter devices in car industries, construction, microelectronics [3].

Consequently, the usage of these industrial materials is expected to increase in developing countries such and Myanmar and others Asia countries. Proper usage of these industrial materials depends on basic research data as well as proper education and knowledge sharing to achieve sustainable and safe industrial development inside Asia as well as global. From this point of view, surface properties of these industrial materials such as elemental states, binding energy and chemical composition become important in international standards.

In this work, the development of spectral data base for (T-M-C) by X-ray photoelectron spectroscopy (XPS) will be presented. The data base spectra were accumulated according to ISO standards measurement procedures and techniques such as binding energy calibration and sample cleaning. Among (T-M-C) materials, VC, HfC and Cr_3C_2 are of high possibility for many applications in future industry due to their unique physical properties like hardness, high melting temperature and high thermal expansion coefficient [4, 5]. Spectral analysis for database of these materials will be discuss in detail.

Surface Science and Nanotechnology

Thithi Lay, M. Imamura[*2], N. Matsubayashi[*2] (*1 National Institute of *Advanced Industrial Science and Technology* (*AIST*))
Proceedings of the 1st International conference on Recent Innovations in Nanoscience and Technology" 333-336 (2018)

Recent development in nanotechnology is closely related to surface science through scientific disciplines, phenomena, measurement tools & techniques. Surface science cover wide range of research and development such as semiconductor, microelectronics, sensor, molecular science etc. Nanoscales research strongly related with surface analysis which include morphology, material structure, chemical bonding, optical and mechanical properties. A few examples will be given mainly from work performed to highlight thin film, surface and interface analysis.

標準化データベース用金属化合物の分析
Surface Analysis of Metal Compounds for Standard Database

Thithi Lay
Josai Information Sciences Researches **27**, 44-49 (2020)

光電子分光装置エネルギー軸較正法（ISO 15472）の測定手順に沿って光電子分光装置PHI5500（ULVAC-PHI 社）の結合エネルギー軸の目盛りの直線性を確認した。較正用標準試料として金，銀，銅を用いて測定し，得られた測定データの計算結果から特定のピーク位置で観察されたエネルギーの直線性誤差 ε_2 は信頼度 95% で較正されたエネルギー軸目盛りの確からしさ U^1_{95}（誤差範囲）よりも小さい（ε_2=0.0065 ＜ U^1_{95}=0.0475）値が得られた。測定結果から装置の結合エネルギー軸目盛りは直線的であり標準データベースを目的とする測定が可能であることが分かった。利用する測定装置の信頼性が得られたため，工業用材料の標準データベースを目的としてハフニウムカーバイト（HfC）のスペクトル分析を行ったのでその結果について報告する。

2. Books, Reviews and Other Printings

MATHEMATICS

計算尺を使った数学教育
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講究録
2067（2018），1-10.

Fuch 型方程式の接続問題
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講究録 2101（2019），98-118.

多面体からできる回転体の教材作成とその利用について
濱口直樹，大島利雄，高遠節夫
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講究録
2105（2019），19-25.

個数を数える
大島利雄
数学書房，226 pp，2019.

中高生向けの数学の講義の工夫
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講究録
2142（2020），1-10.

Proceedings of the Meeting for Study of Number Theory, Hopf Algebras and Related Topics.
Held in Toyama, February 12-15, 2017. Edited by Hiroyuki Yamane, Takeyoshi Kogiso, Yoshiyuki Koga and Iwao Kimura. Yokohama Publishers, Yokohama, 2019.
iv+269 pp. ISBN: 978-4-946552-65-6 11-06（16-06 17-06）

数学科サイト上の数式処理ソフト Maple 活用教材のリニューアル
中村俊子，紀藤優太
城西情報科学研究 26（2020），23-29.

MathSchiNet Mathematical Reviews（https://mathscinet.ams.org/mathscinet）
・MR3998716（reviewer : Masatoshi Iida）
・MR4104013（reviewer : Masatoshi Iida）
・MR4153158（reviewer : Masatoshi Iida）

防御対策のためのインフルエンザの流行シミュレーション
安田英典．シミュレーション，38，(2019) 59-62.

トレース不等式から見た不確定性関係Ⅱ
柳研二郎
京都大学数理解析研究所講究録，vol.2095，2018，pp.157-170

Inequalities for tracial positive linear maps related to quantum information theory
Kenjiro Yanagi
実解析学シンポジウム 2018 報告集，vol.50，2018，pp.43-48

量子情報理論におけるトレース型正線型写像に対するいくつかの不等式
柳研二郎
第 41 回情報理論とその応用シンポジウム資料，vol.41，2018，pp.550-555

Uncertainty relations for quantum channels
Kenjiro Yanagi
実解析学シンポジウム 2019 報告集，vol.51，2019，pp.106-112

量子情報理論と不確定性関係
柳研二郎
電子情報通信学会技術研究報告集 , vol.119, no.308, 2019, pp.21-26

量子通信路に関連した一般化 quasi-metric adjusted 歪情報量によって表現された不確定性関係
柳研二郎
第 42 回情報理論とその応用シンポジウム資料，vol.42，2019，pp.227-232

Uncertainty Relations
Kenjiro Yanagi
「Quantum Mechanics」Section 2, Chapter 4, IntechOpen, 2020, pp.47-63

CHEMISTRY

マテリアルズ・インフォマティクス Q&A 集－解析実務と応用事例－
寺前裕之
516-518 情報機構 (2020)

A themed issue of functional molecule-based magnets: Dedicated to Professor Masahiro Yamashita on the occasion of his 65th birthday
Keiich Katoh[*1] (Special Issue Editor) (*1 Tohoku University)
Magnetochemistry, **6**, 1-2 (2020).

有機溶媒系におけるカーボンナノチューブの分離精製
前田優[*1]，山田道夫[*1]，紺野優以[*1]，鈴木光明（*1 Tokyo Gakugei University）
カーボンナノチューブの表面処理・分散技術と複合化事例，（株）技術情報協会，p.69 ～ p.76（2019）.

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，石黒直哉
DNA 多型，**26**, 64-68（2018）.

遺伝子から解き明かす魚の不思議な世界：11 章 魚の卵の膜とそれを分解する酵素の共進化
佐野香織，一色出版 p. 313-349（2019）.

Second-order phase transition behavior in a polymer above the glass transition temperature
Mitsuru Ishikawa, Taihei Takahashi, Yu-ichiro Hayashi, Maya Akashi, Takayuki Uwada
ChemRxiv^{TM} 12696029, DOI 10.26434（July 23, 2020）

ナノスケールにおける沸騰現象
橋本修一*，宇和田貴之（* 群馬工業高等専門学校専攻科）
CSJ カレントレビュー 35 有機・無機材料の相転移ダイナミクス，日本化学会編，pp. 83-92，化学同人（2020）

第２章　オイルゲル化剤の開発と応用事例，第２節　２成分オイルゲル化剤の開発
橋本雅司（2018）
「ゲル化・増粘剤の使い方，選び方　事例集」[（株）技術情報協会]，(137-144).

特許
今野英雄　橋本雅司　特願 2019-182326

Women in Politics
Thin Nandar Hlaing[*1], Thithi Lay（*1 University of Yangon）
Josai Center for ASEAN Studies, Project Research Report（2017）

Gender Discrimination in Women Sport at Josai University（Case Study）
Dianita Candra Dewi[*1], Nur Faqihah Binthi Norizan[*1], May PhyoPaing[*2], ThithiLay（*1 Josai International University, *2 University of Yangon）
Josai Center for ASEAN Studies, Project Research Report（2017）

Women in STEM and Research（Gender Gap）
Yenna Chastine Deliman[*1], Myo Thiri Cho[*2], ThithiLay（*1 Josai International University, *2 University of Yangon）
Josai Center for ASEAN Studies, Project Research Report（2017）

3. Oral Presentations

MATHEMATICS

超幾何微分方程式の解の接続問題
大島利雄
超幾何研究会 2018，神戸大学，2018 年 1 月 6 日.

超幾何微分方程式の解の接続問題
大島利雄
ウィンターセミナー 2018，KKR 水上，2018 年 2 月 4 日.

大学における数学教育の問題点と工夫
大島利雄
教育数学の一側面—高等教育における数学の多様性と普遍性—，京都大学数理科学研究所，2018 年 2 月 14 日.

Hypergeometric equations ¦ connection problem and confluence/unfolding
大島利雄
アクセサリー・パラメータ研究会，熊本大学，2018 年 3 月 15 日.

Risa/Asir の使い勝手の向上
大島利雄
Risa/Asir Conference 2018，金沢大学，2018 年 3 月 25 日.

Hypergeometric equations with several variables ¦ connection problems and confluences
Toshio Oshima
FASPDE18, Padova Univ., June 26, 2018.

能動的学修に向けて ― 数学を楽しく
大島利雄
福島県高等学校数学部会県南支部研修会，須賀川高校，2018 年 5 月 31 日.

計算尺を使った教育 ― 小学生から
大島利雄
幾何学とインターネットの数理 2018, 東京大学玉原セミナーハウス，2018 年 7 月 14 日.

常微分方程式と KZ 方程式の接続問題と合流操作と middle convolution
大島利雄
アクセサリー・パラメータ研究会，玉原国際セミナーハウス，2018 年 8 月 4，5，6 日.

多面体からできる回転体の教材作成とその利用について
濱口直樹，大島利雄，高遠節夫
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，2018 年 8 月 27 日.

Confluence and unfolding of irregular singularities of hypergeometric equations
大島利雄
代数解析学の諸問題 — 超局所解析及び漸近解析 —, 京都大学数理解析研究所，2018 年 10 月 18 日.

From Fuchsian ordinary differential equations on P1 to equations with several variables and irregular singularities
Toshio Oshima
The Legacy of Joseph Fourier after 250 years, Tsingua Sanya International Mathematics Forum, Sanya, China, Dec. 18, 2018.

分かる Fuchs 型常微分方程式から不確定特異点をもつ多変数方程式へ
大島利雄
微分方程式と表現論，城西大学紀尾井町キャンパス，2018 年 12 月 26 日.

接続公式の合流
大島利雄
ウィンターセミナー 2018，KKR 上諏訪，2019 年 2 月 17 日.

Risa/Asir と TeX を用いた教材作成
大島利雄
数学教育セミナー，城西大学紀尾井町キャンパス，2019 年 3 月 2 日.

接続問題の合流と開折
大島利雄
代数解析学の諸問題，日本大学駿河台キャンパス，2019 年 3 月 7 日.

合流と開折 — 接続問題と多変数化
大島利雄
アクセサリー・パラメータ研究会 , 熊本大学，2019 年 3 月 14 日.

Analysis of hypergometric systems via confluence and fractional derivative
Toshio Oshima
Representation theory of reductive Lie algebras, 東京大学大学駒場キャンパス，Mar 28, 2019.

身近に観察できる曲線に潜む数理
大島利雄

東京家政大学附属中学・高校，2019 年 7 月 11 日.

数学研究におけるコンピュータの活用 ― 代数計算および可視化
大島利雄
東京大学玉原セミナーハウス，2019 年 7 月 13 日.

現代の暗号について
大島利雄
山幸政経塾，博多，2019 年 7 月 19 日.

中高校生向けの数学の講義の工夫
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，2019 年 8 月 21 日.

Confluence and Unfolding of Pfaan Systems
Toshio Oshima
FASFE19, Valladolid, Spain, Sep. 10, 2019.

Confluence and Unfolding of Pfaffian Systems
Toshio Oshima
Advances and Perspectives in Representation Theory, Shandong University, Quingdao China, Oct. 15, 2019.

Confluence and versal unfolding of Pfaffian systems
大島利雄
超幾何微分方程式研究会，神戸大学，2020 年 1 月 5 日.

Pfaff 系の合流と開折とその応用
大島利雄
2019 年度表現論ワークショップ，鳥取市県民ふれあい会館，2020 年 1 月 11 日.

Pfaff 系の合流と開折
大島利雄
ウィンターセミナー 2019, KKR 甲府ニュー芙蓉，2020 年 2 月 17 日.

超関数 ― 関数概念の拡張
大島利雄
現代数学への誘い，NHK 文化センター町田教室，2020 年 9 月 19 日.

Recipe for making Kauffman bracket by using cluster algebras of A, B
小木曽岳義

表現論ワークショップ（鳥取市ふれあい会館）2018 年 01 月 – 2018 年 01 月伊師英之

Local functional equations of homaloidal polynomials.
Takeyoshi Kogiso（招待）
Laboratoire de Mathématiques de Reims FRE 2011 du CNRS（Reims University), France, 2018 年 07 月 – 2018 年 07 月 Michael Pevzner

Clifford quartic forms and its applications.
Takeyoshi Kogiso（招待）
Séminaire Théorie de Lie, Géométrie et Analyse（LieGA）（Metz IECL), France, 2018 年 06 月 – 2018 年 06 月 Khalid Koufany

Local functional equations of homaloidal polynomials.
Takeyoshi Kogiso（招待）
Séminaire Théorie de Lie, Géométrie et Analyse（LieGA）（Institut Elie Cartan de Lorraine), France, 2018 年 03 月 – 2018 年 03 月 Khalid Koufany

Snake graph, Conway Coxeter フリーズ，有理絡み目の関係
小木曽岳義（招待）
Knotting Nagoya（名古屋工業大学）2018 年 10 月 – 2018 年 10 月平澤美可三

Cluster algebras and Knot invariants.
Takeyoshi Kogiso（招待）
Hopf algebra theory and related topics,（富山高等専門学校）2019 年 02 月 – 2019 年 02 月山根宏之

団代数と結び目多項式
小木曽岳義
表現論ワークショップ 2019 年 03 月 – 2019 年 03 月伊師英之

Cluster algebras and Knot invariants
Takeyoshi Kogiso（招待）
金沢大学代数学セミナー，（金沢大学）2019 年 07 月 – 2019 年 07 月大浦学

Where do homaloidal polynomials appear?
Takeyoshi Kogiso（招待）
室蘭整数論セミナー，（室蘭工業大学）2019 年 08 月 – 2019 年 08 月桂田英典

***q*-Deformations of continued fractions and Knot polynomials.**
Takeyoshi Kogiso（招待）
トポロジーとコンピュータ 2019（大阪市立大学）2019 年 10 月 – 2019 年 10 月吉田はん

連分数の q- 変形とその応用
小木曽岳義（招待）
早稲田大学整数論セミナー（早稲田大学西早稲田キャンパス 61 号館 4 階 413 室）2019 年 11 月 – 2019 年 11 月成田宏秋

***q*-Deformation of a continued fraction and its applications.**
Takeyoshi Kogiso（招待）
東大数理トポロジー火曜セミナー，（東京大学大学院数理科学研究科）2019 年 12 月 – 2019 年 12 月逆井卓也

連分数の q- 変形と特殊関数
小木曽岳義
表現論ワークショップ（「県民ふれあい会館」（鳥取県立生涯学習センター））2020 年 01 月 – 2020 年 01 月伊師英之

***q*-Deformation of continued fractions and its application to the Markov equation**
Takeyoshi Kogiso
The 2nd Meeting for Number theory, Hopf algebras and related topics,（富山大学五福キャンパス）2020 年 02 月 – 2020 年 02 月 Hiroyuki Yamane

***q*-Deformation of continued fractions and its application to the Markov equation and further generalization.**
Takeyoshi Kogiso（招待）
第 7 回京都保形型形式研究集会（京都大学）2020 年 06 月 – 2020 年 06 月雪江明彦

On the behavior of solutions for Lanchester square-law models with timedependent coefficients
荻原俊子
芝浦工業大学における微分方程式セミナー，芝浦工業大学，2018 年 8 月.

時間に依存した係数を持つ Deitchman モデルの解の挙動について
桑山優希，荻原俊子
2018 年度応用数学合同研究集会，龍谷大学，2018 年 12 月.

Asymptotic behavior of solutions for nonautonomous Lanchester type systems
Toshiko Ogiwara
NCTS 2019 Workshop on Applied Mathematics in Taichung, National Chung Hsing University (Taiwan), 2019 年 3 月.

戦闘モデルに関連した非自励的 2 種競争系の解の挙動
荻原俊子
非線形現象の数理解析，北海道大学，2019 年 3 月.

On the Stokes geometry of a unified family of P_J-hierarchies（J=I,II,IV,34）
Yoko Umeta,
Formal and Analytic Solutions of Partial Differential Equations FASPDE18, Padova University, Italy, 2018 年 6 月

On the Stokes geometry of a unified family of P_J-hierarchies（J=I,II,IV,34）
Yoko Umeta,
Workshop on Algebraic analysis and Asymptotic analysis in Hokkaido, 北海道大学，2018 年 5 月

Recovering a linear problem from a nonlinear problem
Akane Nakamura
Representation Theory and Integrable Systems, ETH, スイス，2019 年 8 月.

Recovering a linear problem from a nonlinear problem
Akane Nakamura
The 2nd International Conference Geometry of Submanifolds and Integrable Systems, 大阪市立大学，2019 年 3 月.

Recovering a linear problem from a nonlinear problem
Akane Nakamura
Kobe Seminar on Integrable Systems, 神戸大学，2019 年 2 月.

Recovering a linear problem from a nonlinear problem
Akane Nakamura
（ポスター）, SIDE 13, 福岡，2018 年 11 月.

Recovering a linear problem from a nonlinear problem
Akane Nakamura
可積分系理論から見える数理構造とその応用，京都大学数理解析研究所，2018 年 9 月.

Generalised Hitchin systems
Akane Nakamura
Seminar on geometric aspects of integrable dynamical systems
山梨県大泉，2018 年 6 月.

The Bäcklund transformations of the matrix Painlevé equations
Akane Nakamura
Asymptotic, Algebraic and Geometric Aspects of Integrable Systems, TSIMF, 中国，2018 年 4 月.

Generalized Hitchin systems and generic degeneration of spectral curves
Akane Nakamura

可積分系ウィンターセミナー，水上，2018 年 2 月.

感染症流行防御のためのシミュレーション
安田英典，鈴木和男.
安全工学シンポジウム 2020 講演予稿集，68-71（日本学術会議 2020/7）. ISSN1342-4432.

BBM 方程式の高精度解法の比較
安田英典.
日本応用数理学会 2019 年会講演予稿集，329-330（東京 2019/9）.

Simulation of influenza A/H5N1 in host.
H.Yasuda
EASIAM 2018,（Tokyo 2018/June）.

トレース不等式から見た不確定性関係Ⅱ
柳研二郎
京都大学数理解析研究所・研究集会（代表者：松岡勝男）
「関数空間の深化とその周辺」，京都大学，京都市，2018 年 2 月

Inequalities for tracial positive linear maps related to quantum information theory
Kenjiro Yanagi
実解析学シンポジウム 2018，大阪教育大学，大阪市，2018 年 11 月

Some kinds of uncertainty relations for generalized quasi-metric adjusted skew informations and their applications
柳研二郎
The 7th International Conference on Nonlinear Analysis and Optimization, Okinawa Institute of Science and Technology Graduate University & ANA International Manza Beach Resort, Okinawa, 2018 年 11 月

量子情報理論におけるトレース型正線型写像に対するいくつかの不等式
柳研二郎
第 41 回情報理論とその応用シンポジウム，スパリゾートハワイアンズ，いわき市，2018 年 12 月

Generalized quasi-metric adjusted skew information based uncertainty relations for quantum channels
Kenjiro Yanagi
International Workshop on Operator Theory and its Applications, University of Lisbon, Portugal, 2019 年 7 月

Uncertainty relations for quantum channels
柳研二郎
実解析学シンポジウム 2019，九州工業大学，北九州市，2019 年 10 月

量子情報理論と不確定性関係
柳研二郎
情報理論研究会：若手研究者のための講演会，霧島国際ホテル，霧島市，2019 年 11 月

量子通信路に関連した一般化 quasi-metric adjusted 歪情報量によって表現された不確定性関係
柳研二郎
第 42 回情報理論とその応用シンポジウム，霧島国際ホテル，霧島市，2019 年 11 月

Uncertainty relations represented by tracial or non-tracial positive linear maps
柳研二郎
京都大学数理解析研究所・研究集会（代表者：松岡勝男）
「関数空間とその周辺」，京都大学，京都市，2019 年 12 月

高頻度データを用いた拡散パラメータの漸進推定手法の考案およびその実装
清水優祐
CREST・さきがけ数学関連領域合同シンポジウム「数学パワーが世界を変える 2018」，アキバホール（東京都千代田区），2018 年 1 月

高頻度データを用いた拡散パラメータの逐次推定手法の考案およびその実装
清水優祐
CREST・さきがけ・AIMaP 合同シンポジウム「数学パワーが世界を変える 2019」，東京ガーデンパレス（東京都文京区），2019 年 3 月

逐次推定を用いた確率微分方程式モデルに対する新たな推定手法の考案および数値実装による実装
清水優祐
城西大学学長所管研究費報告会，城西大学（坂戸キャンパス），2019 年 6 月

確率微分方程式モデルの推定手法について
清水優祐
第 2 回統計科学セミナー，東京理科大学（野田キャンパス），2020 年 11 月

CHEMISTRY

Ab Initio Electronic Structure Calculation of Polymononucleotide, a Model of B-type DNA
Hiroyuki Teramae, Yuriko Aoki[*1]（*1 Kyushu University）
ICCMSE2018（Thessaloniki），2018 年 3 月 , CC Symposium（16）Biology II（invited）

フェルラ酸のフリーラジカル消去能に関する理論的研究
寺前裕之，玄美燕[*1]，山下司[*1]，高山淳[*1]，岡﨑真理[*1]，坂本武史[*1]（*1 城西大薬）
日本コンピュータ化学会 2018 年春季年会（東京），2018 年 6 月，講演要旨集 1O03

Ab Initio Calculation of Polymononucleotide, a Model of B-type DNA
Hiroyuki Teramae, Yuriko Aoki[*1]（*1 Kyushu University）
5th French-Japanese Workshop on Computational Methods in Chemistry（Strasbourg），2018 年 6 月 2 日（invited）

Ab Initio Study of Polymononucleotide as a Model of B-type DNA
Hiroyuki Teramae, Yuriko Aoki[*1]（*1 Kyushu University）
16TH INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY（Menton），B124, 2018 年 6 月

モデル DNA の Hartree-Fock 計算（2）
寺前裕之，青木百合子[*1]（*1 九大）
分子科学討論会 2018（福岡），2018 年 9 月，講演要旨集 4P122

フェルラ酸の抗酸化作用の置換基効果に関する理論的研究
寺前裕之，玄　美燕[*1]，山下　司[*1]，高山　淳[*1]，岡﨑真理[*1]，坂本武史[*1]（*1 城西大薬）
第 41 回ケモインフォマティクス討論会（熊本），2018 年 10 月，講演要旨集 1P09

結晶軌道法によるモデル DNA の電子状態計算
寺前裕之
第二回琉球大学計算科学シンポジウム（沖縄），2018 年 10 月，セッション 6（基調講演）

分子軌道計算と機械学習によるフェルラ酸の抗酸化作用の研究
寺前裕之，玄美燕，山下司，高山淳，岡﨑真理，坂本武史
日本コンピュータ化学会 2019 年秋季年会（広島），2019 年 10 月，講演要旨集 2O01

機械学習と分子軌道計算を用いた薬物の物性予測
寺前裕之，玄　美燕[*1]，山下　司[*1]，高山　淳[*1]，岡﨑真理[*1]，坂本武史[*1]（*1 城西大薬）
第 42 回ケモインフォマティクス討論会（東京），2019 年 10 月，講演要旨集 1B04

機械学習と分子軌道計算を用いた物性予測
寺前裕之，玄　美燕[*1]，山下　司[*1]，高山　淳[*1]，岡﨑真理[*1]，坂本武史[*1]（*1 城西大薬）
第 47 回構造活性相関シンポジウム（熊本），2019 年 11 月，講演要旨集 1O-04

Possible Prediction of Molecular Properties with Machine Learning and Molecular Orbital Energies
Hiroyuki Teramae, Xuan Meiyan, Tsukasa Yamashita, Jun Takayama, Mari Okazaki, Takeshi Sakamoto

ISENT2019（Yangon), December 2019（Invited）

塩素系有機溶媒中のメタノール－ピリジン水素結合会合体の水素結合エネルギー
二見能資[*1]，尾﨑　裕，尾崎幸洋[*2]（*1 熊本高専，*2 関西学院大）
第 12 回分子科学討論会（福岡），2018 年 9 月

Three-Body Effects on the CO_2 Vibrational Frequency in van der Waals Trimers CO_2-M_2 (M=Kr, Xe, N_2) Investigated by Infrared Diode Laser Spectroscopy
Yasushi Ozaki
ICRINT2018（University of Yangon, Myanmar），December 2018.

Solvent dependence of hydrogen bond energy of methanol-pyridine complex and absorption intensity of fundamental and overtone of OH stretching vibration of methanol monomer
Yoshisuke Futami[*1], Yasushi Ozaki, Yukihiro Ozaki[*2]（*1 熊本高専，*2 関西学院大）
日本化学会第 99 春季年会 4A3-03（神戸），2019 年 3 月

フレキシブル色素増感太陽電池に用いる TiO_2 光電極の作製と評価
柴山　巧，見附孝一郎
web 光化学討論会，2020 年 9 月，講演要旨集，1P-096

気／水界面上の C_{60} 脂肪酸混合薄膜とその LB 転写膜における C_{60} の分散状態
小澤奈々子・田沼佑里・見附孝一郎
日本化学会第 100 春季年会（野田），2020 年 3 月，講演要旨集，2PB-125

Analyses of parameters affecting the fill factors of dye sensitized solar cells
Koichiro Mitsuke, Ryohei Watai, Katsunari Takuma, Takumu Fujiya
International Symposium on Environmental-Life Science and Nanoscales Technology 2019 (ISENT2019), Yangon, 2019 年 12 月

Temperature dependence of the current-voltage characteristics of organic solar cells
Katsunari Takuma, Ryohei Watai, Takumu Fujiya, Ayano Higashimura, Koichiro Mitsuke
35th Symposium on Chemical Kinetics and Dynamics（Higashi-Hiroshima), 2019 年 6 月，Book of Abstracts, 2P23

ペロブスカイト接合面におけるエキシトンの電荷分離
齋藤祐希，出島康琢，東村綾乃，見附孝一郎
第 12 回分子科学討論会（福岡），2018 年 9 月，講演要旨集，4P-054

Impedance analyses for the interface of nanostructures in dye-sensitized solar cells
Ryohei Watai, Takumu Fujiya, Koichiro Mitsuke
34th Symposium on Chemical Kinetics and Dynamics（Kizugawa），2018 年 6 月，Book of

Abstracts, 2P07

Exciton dissociation to charge carriers in perovskite solar cells
Yuki Saito, Koichiro Mitsuke
34th Symposium on Chemical Kinetics and Dynamics (Kizugawa), 2018 年 6 月, Book of Abstracts, 2P08

Transient emission spectroscopy of dye molecules adsorbed on metal oxide semiconductor
Koichiro Mitsuke, Kohei Watanabe, Kohei Takayanagi, Akira Yoshida
日本化学会第 98 春季年会（船橋), 2018 年 3 月, 講演要旨集, 1PC-015

Photoelectron Spectroscopy of Endohedral Fullerenes
H. Yagi, T. Zaima[*1], S. Okita[*1], Y. Seino[*1], T. Miyazaki[*1], H. Shinohara[*2], S. Hino[*1] (*1 Ehime University, *2 Nagoya University)
International Symposium on Environmental Life Science and Nanoscales Technology, 2019 (Yangon), 2019 年 12 月

Solution structural analysis of novel small heat shock protein Orf7.5 from *Synechococcus elongatus* PCC 7942.
H. Morita, N. Omiya, N. Ishikawa, N. Tanaka, H. Hayashi, H. Nakamoto
XXVIIIth International Conference on Magenetic Resonance in Biological System (Dublin, Ireland), 2018 年 8 月

好冷性細菌 *Anabaena variabilis* 由来のグリシンリッチドメインを持たない RNA 結合タンパク質 RbpD の溶液構造の特徴
森田勇人, 田中邑樹, 古板恭子, 杉木俊彦, 児嶋長次郎
第 59 回 NMR 討論会（2020), 2020 年 11 月, 講演要旨集, 2L6

臭化銅（I）イソシアニド錯体の発光特性
南山知花, 髙木　衛, 早川拓弥, 阪田知巳
第 65 回応用物理学会春季学術講演会（東京), 2018 年 3 月, 講演要旨集 17p-P6-18

銅（I）イソシアニド錯体における発光特性の温度依存性
南山知花, 髙澤頼昌, 阪田知巳
第 79 回応用物理学会秋季学術講演会（名古屋), 2018 年 9 月, 講演要旨集 20p-PA2-5

銅（I）イソシアニド錯体のサーモクロミズム
南山知花, 髙澤頼昌, 阪田知巳
第 35 回「センサ・マイクロマシンと応用システム」シンポジウム（札幌), 2018 年 10 月, 講演要旨集 30am3-P5-55

アニール処理よる臭化銅（I）錯体の可逆的メカノクロミズム
南山知花，髙澤頼昌，阪田知巳
第 66 回応用物理学会春季学術講演会（東京），2019 年 3 月，講演要旨集 9a-PA2-38

Luminescent Properties of Copper（I)-bromide Complex in a PMMA Film
C. Nanzan, Y. Takazawa, T. Sakata
EM-NANO 2019，2019 年 6 月，講演要旨集 P1-5, Shinshu University

Molecular Compounds Comprising 3′-Aminofluorene-9-spiro-5′-imidazolidine -2′,4′-dithione
Y. Takazawa, T. Yamamoto, T. Sakata
ICNI 2019，2019 年 9 月，講演要旨集 P87, University of Lisbon

臭化銅（I）イソシアニド錯体を含有する PMMA 薄膜の可逆的発光性メカノクロミズム
南山知花，髙澤頼昌，阪田知巳
第 80 回応用物理学会秋季学術講演会（札幌），2019 年 9 月，講演要旨集 20p-PA3-18

銅（I）イソシアニド錯体を含有する PMMA 薄膜の光学特性
南山知花，髙澤頼昌，阪田知巳
第 36 回「センサ・マイクロマシンと応用システム」シンポジウム（浜松），2019 年 11 月，講演要旨集 21pm-PS3-31

カルボキシエチルホスフィンを配位子とする CuI 錯体の発光特性
髙澤頼昌，南山知花，阪田知巳
第 67 回応用物理学会春季学術講演会（東京），2020 年 3 月，講演要旨集 14p-PB7-14

（2- カルボキシエチル）ジフェニルホスフィンを配位子とするヨウ化銅（I）錯体における発光の温度依存性
髙澤頼昌，阪田知巳
第 81 回応用物理学会秋季学術講演会（オンライン），2020 年 9 月，講演要旨集 8a-Z13-1

OLED の白色化に向けた（2- カルボキシエチル）ジフェニルホスフィンを配位子とするヨウ化銅（I）錯体の作製
髙澤頼昌，阪田知巳
第 37 回「センサ・マイクロマシンと応用システム」シンポジウム（オンライン），2020 年 10 月，講演要旨集 27P3-SSP-5

2,2′-biimidazole 配位子を持つ［Pb（$C_6H_6N_4$）Cl］［$PbCl_3$］の合成と構造
渡邉佳乃子，鈴木光明，宮前　博
日本化学会第 100 春季年会（講演予稿集），2020 年 3 月，講演要旨集，1PA-110.

Isolation and characterization of higher endohedral metallofullerenes encapsulating La atom
Takuya Adachi, Mitsuaki Suzuki
日本化学会第 100 春季年会（講演予稿集），2020 年 3 月，講演要旨集，1PB-057.

Crystal structure of 2,4-dimethyl-1,5-benzodiazepinium hydrogen sulfate
Ryota Ishikawa, Katsuya Uchida, Mitsuaki Suzuki
日本化学会第 100 春季年会（講演予稿集），2020 年 3 月，講演要旨集，2PB-142.

Simple and Effective Method to Control Photoluminescence Properties of Single-walled Carbon Nanotubes by Ultrasonic Irradiation
Yui Konno[*1], Akane Nishino[*1], Michio Yamada[*1], Yutaka Maeda[*1], Saki Okudaira[*2], Yuhei Miyauchi[*2], Kazunari Matsuda[*2], Jun Matsui[*3], Masaya Mitsuishi[*4], Mitsuaki Suzuki（∗1 Tokyo Gakugei University, ∗2 Kyoto University, ∗3 Yamagata University, ∗4 Tohoku University）
The 58th Fullerenes-Nanotubes-Graphene General Symposium, Tokyo, 2020 年 3 月， Abstract, 2P-1.

Co-crystal of La@C_s(6)-C_{82} with Ni(OEP)
Mitsuaki Suzuki, Takahiro Tanaka, Takuya Adachi, Michio Yamada[*1], Yutaka Maeda[*1], Zdenek Slanina[*2], Shigeru Nagase[*3], and Takeshi Akasaka[*2,4,5]（∗1 Tokyo Gakugei University, ∗2 Huazhong University of Science and Technology, ∗3 Kyoto University, ∗4 Foundation for Advancement of International Science, ∗5 University of Tsukuba）
18th International Symposium on Novel Aromatic Compounds, Sapporo, 2019 年 7 月, Abstract, Poster-072.

Platinum-catalyzed reaction of [60] fullerene with 9-Ethynyl-9*H* -fluoren-9-yl carboxylates
Mayu Takizawa[*1], Yoko Nukatani[*1], Mitsuaki Suzuki, Yutaka Maeda[*1], Michio Yamada[*1]（∗1 Tokyo Gakugei University）
The 56th Fullerenes-Nanotubes-Graphene General Symposium, Tokyo, 2019 年 3 月， Abstract, 3P-1.

Temperature dependence of anisotropic transient conductivity of a La@C_{2v}-C_{82}(Ad) crystal
Michio Yamada[*1], Satoru Sato[*2], Wookjin Choi[*3], Shu Seki[*3], Tsuneyuki Abe[*2], Mitsuaki Suzuki, Yutaka Maeda[*1], Shigeru Nagase[*3], Takeshi Akasaka[*1,2,4,5]（∗1 Tokyo Gakugei University, ∗2 University of Tsukuba, ∗3 Kyoto University, ∗4 Foundation for Advancement of International Science, ∗5 Huazhong University of Science and Technology）
The 54th Fullerene-Nanotube-Graphene General Symposium, Tokyo, 2018 年 3 月， Abstracts, 1P-2.

La@C_s(6)-C_{82} と Ni(OEP) の共結晶化
安達拓哉，田中貴大，鈴木光明，山田道夫[*1]，前田　優[*1]，Zdenek Slanina[*2]，永瀬　茂[*3]，赤阪

健[*4,5]（*1 東学芸大教，*2 国立中正大学，*3 京大福井セ，*4 FAIS，*5 筑波大 TARA セ）
第 29 回基礎有機化学討論会（東京），2018 年 9 月，講演要旨集，2P015.

C_{60} 還元体を用いたメタノフラーレン合成
山納真人[*1]，坂本航大[*1]，鈴木光明，山田道夫[*1]，前田　優[*1]（*1 東学芸大教）
第 29 回基礎有機化学討論会（東京），2018 年 9 月，講演要旨集，1P018.

Microheterogeneity for calamus of pigeon feather keratin
高橋理恵子
第 91 回 日本生化学会大会（京都），2018 年 9 月，講演要旨集，2P-242

ハト羽毛ケラチン calamus の microheterogeneity
高橋理恵子
第 92 回 日本生化学会大会（横浜），2019 年 9 月，講演要旨集，3P-245

ハト羽毛ケラチン calamus の microheterogeneity
高橋理恵子
第 93 回 日本生化学会大会（オンライン），2020 年 9 月，講演要旨集，P-476

ギフチョウ属の食草選択に関わる遺伝子の同定Ⅱ
北川浩子
第 91 回日本生化学会（京都），2018 年 9 月，2P-245

ギフチョウにおける化合物結合タンパク質（CSP）遺伝子の解析
北川浩子
第 92 回日本生化学会（京都），2019 年 9 月，3P-246

ギフチョウ属の前脚ふ節における食草選択関連遺伝子の同定
北川浩子
第 93 回日本生化学会（京都），2020 年 9 月，P-477

LAMP 法を用いた環境 DNA による在来種－外来種群判別法の開発
石黒直哉
第 10 回 LAMP 研究会（東京），2018 年 2 月

LAMP 法を用いた淡水エビの在来種－外来種群判別法の確立
齊藤達也，石黒直哉
第 1 回環境 DNA 学会　東京大会（東京），2018 年 9 月

環境 DNA 分析にも有効なスナヤツメ隠蔽種判別法の確立
石黒直哉，高山晃徳，金澤　光[*1]（*1 埼玉県環境科学国際センター）
DNA 鑑定学会第 11 回大会（横浜），2018 年 11 月

環境 DNA を用いたアベサンショウウオ（*Hynobius abei*）の分布とその生息域におけるアメリカザリガニの侵入調査
日和佳政[*1]，鈴木裕士，藤長裕平[*1]，石黒直哉（*1 越前市産業環境部）
日本 DNA 多型学会第 27 回学術集会（松江），2018 年 12 月

環境 DNA を用いたゲンジボタルの地域個体群判別法の確立と比較
齊藤達也，石黒直哉
日本 DNA 多型学会第 27 回学術集会（松江），2018 年 12 月

LAMP 法を用いた在来種・外来種群判別法の開発－環境 DNA への適用－
石黒直哉
第 11 回 LAMP 研究会（東京），2019 年 2 月

環境 DNA 分析を用いたカミツキガメ検出系の確立
石黒直哉，甚野訓章，加藤英明[*1]（*1 静大）
日本 DNA 多型学会第 28 回学術集会（京都），2019 年 11 月

環境 DNA 分析を用いた越前市における希少淡水魚類の生息状況調査
日和佳政[*1]，高橋和良，藤長裕平[*1]，石黒直哉（*1 越前市産業環境部）
日本 DNA 多型学会第 28 回学術集会（京都），2019 年 11 月

元荒川上流域におけるムサシトミヨ環境 DNA の動態調査
石黒直哉，韮塚悠貴
日本 DNA 多型学会第 29 回学術集会（東京），2020 年 11 月

リアルタイム PCR 及びデジタル PCR を用いたアベサンショウウオの検出手法の確立
日和佳政[*1]，吉井瑠星，田村祐佳，石黒直哉（*1 ローカル SD クリエーション）
日本 DNA 多型学会第 29 回学術集会（東京），2020 年 11 月

リアルタイム PCR を用いた坂戸市多和目地区の水路および高麗川本流のホトケドジョウ環境 DNA の検出
石黒直哉，増田拓巳
日本 DNA 多型学会第 29 回学術集会（東京），2020 年 11 月

非モデル生物をつかった基礎研究～卵が教えてくれるサカナの進化～
佐野香織
招待講演 , 城西大学 薬学研究科 先端特論 , 2018 年 6 月

さかなの卵の進化 ～ 薄い卵膜と厚い卵膜。それを軟化する酵素と可溶化する酵素 ～
招待講演，長崎大学　水産学部　長崎最西端　進化生態学セミナー，2018 年 9 月

水産資源を守る卵膜の構造進化の理解
文科省　私学事業部　若手勉強会，2019 年 7 月

孵化酵素遺伝子と卵膜遺伝子の共進化がもたらした魚類の多様な孵化機構
シンポジウム：魚類の繁殖～多様すぎる形態と生理に分子生物学のメスを入れる～
佐野香織，川口眞理，安増茂樹
日本動物学会（大阪），2019 年 9 月，要旨集 P26

蛍光単一分子プローブで眺めた高分子緩和時間の特異性
石川　満
第 32 回光ものづくりセミナー
京都府中小企業技術センター（京都市）2020 年 12 月

高分子のガラス転移温度近傍における二次相転移的挙動
石川　満，高橋泰平，林雄一郎，明石真夜，宇和田貴之
2020 年光化学討論会（オンライン）2020 年 9 月

Dynamics of pseudo second-order phase transition behavior in polymer melt disclosed by single molecule spectroscopy
Mitsuru Ishikawa, Taihei Takahashi, Takayuki Uwada
日本化学会　第 100 春季年会（東京理科大・野田キャンパス），2020 年 3 月

フォトンアップコンバージョン発現を目指した二成分分子結晶ナノ粒子の調製と分光測定
宇和田貴之，久保典孝，石川　満，橋本雅司
日本化学会　第 100 春季年会（東京理科大・野田キャンパス），2020 年 3 月

Pseudo second-order phase transition behaviour in polymer melt disclosed by single molecule spectroscopy
Mitsuru Ishikawa
International Symposium on Environmental Life Science and Nanoscales Technology 2019（ISENT 2019）（Yangon, Myanmar）2019 年 12 月（Plenary talk）

Collective polymer motion near the glass-transition temperature disclosed by single-molecule fluorescence spectroscopy beside thermal analysis
Mitsuru Ishikawa, Taihei Takahashi, Yu-ichiro Hayashi, Takayuki Uwada
2019 年光化学討論会（名古屋）2019 年 9 月

タンパク質結晶細孔を反応場とした金ナノ構造体形成
宇和田貴之，河野航平，石川　満
2019 年光化学討論会（名古屋）2019 年 9 月

Disclosing collective motion of a polymer above glass transition temperature by single molecule spectroscopy
Mitsuru Ishikawa, Taihei Takahashi, Yu-ichiro Hayashi, Takayuki Uwada
日本化学会 第 99 春季年会（神戸）, 2019 年 3 月

Fluorescence image analysis of single molecules at polymer/substrate interfaces
Ishikawa Mitsuru, Takahashi Taihei, Hayashi Yuichiro, Uwada Takayuki
日本化学会第 98 春季年会（船橋）2018 年 3 月

蛍光単一プローブを用いた高分子薄膜のガラス転移温度近傍における動的挙動の観測
石川　満，高橋泰平，宇和田貴之
2018 年光化学討論会（西宮）2018 年 9 月

Disclosure of collective motion in polymer above glass transition temperature by single molecule spectroscopy
Mitsuru Ishikawa, Taihei Takahashi, Yu-ichiro Hayashi, Takayuki Uwada
International Conference on Recent Innovations in Nanoscience & Technology 2018（ICRINT 2018）（Yangon, Myanmar）Invited 2018 年 12 月

タンパク質結晶のナノ細孔材料・ナノ反応容器への展開
宇和田貴之
有機分子有機結晶セミナー，群馬工業高等専門学校（群馬），2020 年 6 月 25 日

線維化インスリン投与部位での薬物吸収性の解析
大野由依*，関　智宏*，小島　裕*，三木涼太郎*，細谷　治*，江川祐哉*，宇和田貴之，加園恵三*，関　俊暢*（* 城西大学薬学部薬学科）
日本薬学会第 140 年会，国立京都国際会館（京都），2020 年 3 月，27Y-am10S.

フォトンアップコンバージョン発現を目指した二成分分子結晶ナノ粒子の調製と分光測定
宇和田貴之，久保典孝，石川　満，橋本雅司
日本化学会 第 100 春季年会，日本大学船橋キャンパス（千葉），2020 年 3 月，4D3-35.

Absorption and fluorescence microspectroscopic study of protein crystals as nanoporous materials
Takayuki Uwada
10th Asian Photochemistry Conference（APC 2018）, Howard Civil Service International House（Taipei, Taiwan），2018 年 12 月，S27-C-1.

多孔質材料としてのタンパク質結晶の吸収・蛍光顕微分光
宇和田貴之，河野航平，石川　満
2018 年光化学討論会 , 関西学院大学上ヶ原キャンパス（兵庫），2018 年 9 月，1B04.

プラズモン加熱による液－液相分離の観測と機構解明
相原一生*，池田優也*，宇和田貴之，古部昭広*，橋本修一*（* 徳島大学工学部光応用工学科）
2018 年光化学討論会，関西学院大学上ヶ原キャンパス（兵庫），2018 年 9 月，1D20.

タンパク質結晶への分子の浸透拡散過程の蛍光分光イメージング
宇和田貴之，高橋 郁也，石川　満
日本化学会 第 98 春季年会，日本大学船橋キャンパス（千葉），2018 年 3 月，2F6-14.

アズレンアミド誘導体の合成とその薬理活性
齋藤昇平，今成伽奈，若林英嗣，奥平准之*1，坂上　宏*1（*1 城西大院理・明海大歯）
日本化学会　第 8 回 CSJ 化学フェスタ 2018 船堀　2018 年 10 月 講演要旨集，P8-037

アズレン環の 1,2 位で置換した新規クラウンエーテルの合成とその性状
手塚颯太，鈴木光明，若林英嗣（城西大院理）
日本化学会 第 9 回 CSJ 化学フェスタ 2019 船堀 2019 年 10 月 講演要旨集，P9-045

ソルボサーマル法による一次元ナノチャネルを有する金属ポルフィリン超分子の合成と構造決定
安達裕紀，秋田素子
第 8 回 CSJ 化学フェスタ 2018（東京）2018 年 11 月

固体で赤色蛍光を示すアセナフトイミダゾール誘導体の合成・構造と発光挙動
野口佳世，宇和田貴之，秋田素子
第 8 回 CSJ 化学フェスタ 2018（東京）2018 年 11 月

ガルビノキシル部位でパラ三置換したトリフェニルアミンの合成
浅子雄太，秋田素子
第 12 回有機π電子系シンポジウム（滋賀）2018 年 12 月

Organic Radical - Transition Metal Magnetic Coordination Polymers
Shoya Sato and Motoko Akita
ICRINT2018,（Invited）（Yangon, Myanmar）2018 年 12 月

5,15- ジ（4- ピリジル）-10,20- ジアリールポルフィリンからなる多孔性配位高分子の吸脱着挙動
安達裕紀，秋田素子
第 9 回 CSJ 化学フェスタ 2019（東京）2018 年 11 月

Crystal Structure and Magnetic Properties of Molecule based Magnet composed of organic free radical.
Motoko Akita
ISENT2019,（Yangon, Myanmar）2019 年 12 月

チオフェン環を有するビスフェナントロイミダゾール類の合成・構造・物性
堀越穂高，山﨑真帆，植野啓志，秋田素子
日本化学会第 100 春季年会（野田），2020 年 3 月，開催中止

フェニルトリアゾール骨格を発光性配位子として有する深青色燐光イリジウム錯体
若槻大輔・橋本雅司・今野英雄・小池和英
日本化学会　第９９回春季年会　（甲南大）2019 年 3 月

Synthesis of $KNbO_3$ films on $LiTaO_3$ single crystal by hydrothermal method for lead free high efficiency piezoelectric sensor
Thithi Lay, May Phyo Paing[*1], Khin Phyu Phyu Sin[*1], Khin Khin Win [*1], Ye Chann [*1], Chan Nyein Aung [*1] (*1 University of Yangon)
International Conference on Energy, Materials and Photonics EMP20, (*Oral*) 2020 年 12 月

Thermal Stability of Piezoelectric Materials at High Temperature
Thithi Lay
Proceedings of the International Symposium on Environmental-Life Science and Nanoscales Technology 2019 (*ISENT2019*), 2019 年 12 月

Spectral Analysis of Transition Metal Carbides for Sustainable Industrial Development
Thithi Lay, M. Imamura[*1], N. Matsubayashi[*1], M. Jo[*1], Khin Khin Win [*2] (*1 National Institute of *Advanced Industrial Science and Technology* (*AIST*), *2 University of Yangon)
Proceedings of the 19th. Science Council of Asia (*SCA*) *Conference,* (*Research and Innovation for Sustainable Development in Asia, 2019*) (*Oral*), 2019 年 12 月

Surface Science and Nanotechnology
Thithi Lay, M. Imamura[*1], N. Matsubayashi[*1] (*1 National Institute of *Advanced Industrial Science and Technology* (*AIST*))
1st International conference on Recent Innovations in Nanoscience and Technol. (*Oral*), 2018 年 12 月

Recent Development of Healthcare: Cosmetic and Pharmaceutical in ASEAN Countries
Thithi Lay, Kenji Sugibayashi
The 1st International conference on Halal Pharmaceuticals and Cosmetics (*HPC*) (*Oral*) 2018 年 12 月

Surface and Interfacial Reaction of Al2O3/SiO2/Si films by SR-XPS
Thithi Lay, M. Imamura[*1], N. Matsubayashi[*1], M. Jo[*1] (*1 National Institute of *Advanced Industrial Science and Technology* (*AIST*))
5th Ito International Research Center Conference (*IIRC5*) *in Tokyo, Japan* (*Poster*), 2017 年 11 月

Science Bulletin of Josai University
Vol. 25 （2021）

Published by Faculty of Science,
Josai University,
Sakado, Saitama 350-0295 Japan

城西大学理学部研究報告
第 25 巻（令和 3 年）

編集・発行　城西大学理学部
〒 350-0295　埼玉県坂戸市けやき台 1-1
Tel.　049-271-7728
編 集 委 員　尾崎　　裕（委員長）
中村　あかね　寺前　裕之
伊藤　　陽

㈱ 外 為 印 刷
印　刷　所　〒111-0032　東京都台東区浅草 2-28-31
Tel.　03-3844-3855（代）